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NEWS 4 OCT 30 CHEMLIST enhanced with new search and display field  
NEWS 5 NOV 03 JAPIO enhanced with IPC 8 features and functionality  
NEWS 6 NOV 10 CA/Caplus F-Term thesaurus enhanced  
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NEWS 8 NOV 20 CA/Caplus to MARPAT accession number crossover limit increased  
to 50,000  
NEWS 9 DEC 01 CAS REGISTRY updated with new ambiguity codes  
NEWS 10 DEC 11 CAS REGISTRY chemical nomenclature enhanced  
NEWS 11 DEC 14 WPIDS/WPINDEX/WPIX manual codes updated  
NEWS 12 DEC 14 GBFULL and FRFULL enhanced with IPC 8 features and  
functionality  
NEWS 13 DEC 18 CA/Caplus pre-1967 chemical substance index entries enhanced  
with preparation role  
NEWS 14 DEC 18 CA/Caplus patent kind codes updated  
NEWS 15 DEC 18 MARPAT to CA/Caplus accession number crossover limit increased  
to 50,000  
NEWS 16 DEC 18 MEDLINE updated in preparation for 2007 reload  
NEWS 17 DEC 27 CA/Caplus enhanced with more pre-1907 records  
NEWS 18 JAN 08 CHEMLIST enhanced with New Zealand Inventory of Chemicals  
NEWS 19 JAN 16 CA/Caplus Company Name Thesaurus enhanced and reloaded  
NEWS 20 JAN 16 IPC version 2007.01 thesaurus available on STN  
NEWS 21 JAN 16 WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data  
NEWS 22 JAN 22 CA/Caplus updated with revised CAS roles  
NEWS 23 JAN 22 CA/Caplus enhanced with patent applications from India  
NEWS 24 JAN 29 PHAR reloaded with new search and display fields  
NEWS 25 JAN 29 CAS Registry Number crossover limit increased to 300,000 in  
multiple databases  
NEWS 26 FEB 13 CASREACT coverage to be extended  
NEWS 27 Feb 15 PATDPASPC enhanced with Drug Approval numbers  
NEWS 28 Feb 15 RUSSIAPAT enhanced with pre-1994 records

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MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

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FILE 'HOME' ENTERED AT 15:01:17 ON 22 FEB 2007

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 15:01:24 ON 22 FEB 2007  
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STRUCTURE FILE UPDATES: 22 FEB 2007 HIGHEST RN 922553-43-3  
 DICTIONARY FILE UPDATES: 22 FEB 2007 HIGHEST RN 922553-43-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

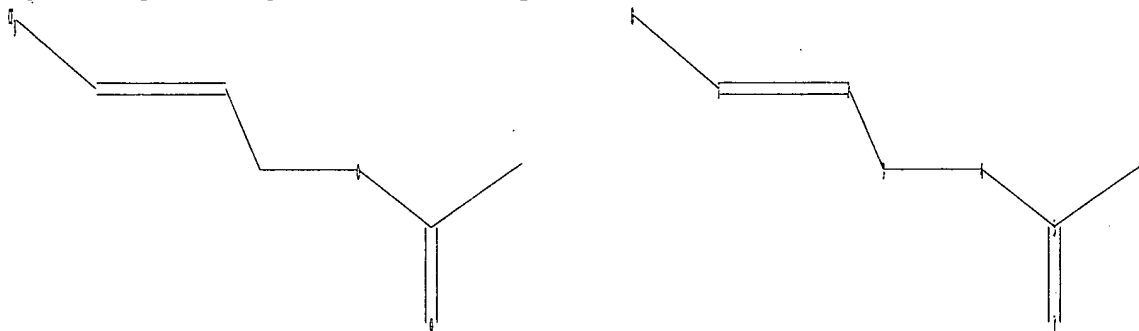
TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

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=>  
 Uploading C:\Program Files\Stnexp\Queries\10539639\Struc 3.str



chain nodes :

10539639a.trn

Page 3

1 2 3 4 5 6 7 8  
chain bonds :  
1-2 1-8 2-3 3-4 4-5 5-6 5-7  
exact/norm bonds :  
3-4 4-5 5-7  
exact bonds :  
1-2 1-8 2-3 5-6

Match level :

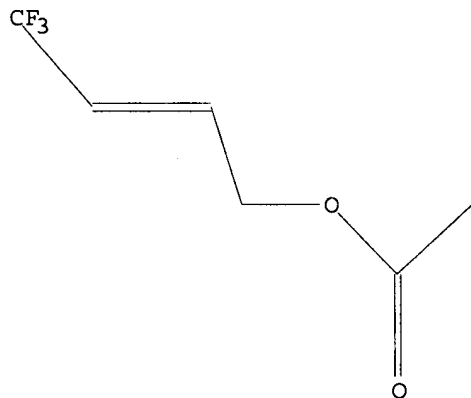
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> l1

SAMPLE SEARCH INITIATED 15:01:35 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 355 TO ITERATE

100.0% PROCESSED 355 ITERATIONS -

4 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 5970 TO 8230

PROJECTED ANSWERS: 4 TO 200

L2 4 SEA SSS SAM L1

=> l1 full

FULL SEARCH INITIATED 15:01:38 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 6551 TO ITERATE

100.0% PROCESSED 6551 ITERATIONS

85 ANSWERS

SEARCH TIME: 00.00.01

10539639a.trn

L3 85 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	172.10	172.31

FILE 'CAPLUS' ENTERED AT 15:02:01 ON 22 FEB 2007  
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FILE COVERS 1907 - 22 Feb 2007 VOL 146 ISS 9  
 FILE LAST UPDATED: 21 Feb 2007 (20070221/ED)

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=> l3

L4 42 L3

=> file reg

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	ENTRY	SESSION
FULL ESTIMATED COST	0.47	172.78

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 DICTIONARY FILE UPDATES: 22 FEB 2007 HIGHEST RN 922553-43-3

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of

10539639a.trn

experimental property data in the original document. For information on property searching in REGISTRY, refer to:

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=> l1 exa

SAMPLE SEARCH INITIATED 15:02:21 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 2 TO 124

PROJECTED ANSWERS: 0 TO 0

L5 0 SEA EXA SAM L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.45

173.23

FILE 'CAPLUS' ENTERED AT 15:02:32 ON 22 FEB 2007

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=> d l4 ibib abs hitstr 1-42

L4 ANSWER 1 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:692963 CAPLUS  
 DOCUMENT NUMBER: 145:292620  
 TITLE: Preparation of CF<sub>3</sub>-containing 1,3-di- and 1,1,3-trisubstituted allenes  
 AUTHOR(S): Yamazaki, Takashi; Yamamoto, Takahiro; Ichihara, Ritsuko  
 CORPORATE SOURCE: Strategic Research Initiative for Future Nano-Science and Technology, Institute of Symbiotic Science and Technology, Tokyo University of Agriculture and Technology, 2-24-16 Nakamachi, Koganei, 184-8588, Japan  
 SOURCE: Journal of Organic Chemistry (2006), 71(16), 6251-6253  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 145:292620  
 AB Novel synthetic pathway to access trifluoromethylated allenes with 1,3-di-

as well as 1,1,3-trisubstitution patterns was developed from a variety of 4,4,4-trifluorobut-2-yn-1-ols which were then transformed into the corresponding vinylic iodides in highly regio- and stereospecific manners.

and zinc-mediated  $\beta$ -elimination after trifluoroacetylation of the hydroxyl group eventually realized the formation of the target mols. in good to excellent overall yields in facile and short steps.

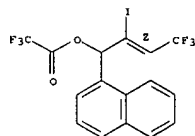
IT 908608-97-9P 908608-98-0P 908609-00-7P  
 908609-01-8P 908609-04-1P 908609-05-2P  
 908609-07-4P 908609-08-5P 908609-09-6P  
 908609-10-9P 908609-11-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of CF<sub>3</sub>-containing 1,3-di- and 1,1,3-trisubstituted allenes from

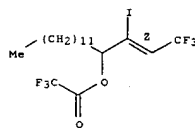
4,4,4-trifluorobut-2-yn-1-ols)

RN 908608-97-9 CAPLUS  
 CN Acetic acid, trifluoro-, (2Z)-4,4,4-trifluoro-2-iodo-1-(1-naphthalenyl)-2-butenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

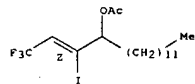


L4 ANSWER 1 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



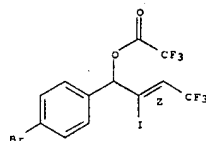
RN 908609-05-2 CAPLUS  
 CN 2-Hexadecen-4-ol, 1,1,1-trifluoro-3-iodo-, acetate, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 908609-07-4 CAPLUS  
 CN Acetic acid, trifluoro-, (2Z)-1-(4-bromophenyl)-4,4,4-trifluoro-2-iodo-2-butenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



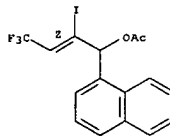
RN 908609-08-5 CAPLUS  
 CN Acetic acid, trifluoro-, (2Z)-4,4,4-trifluoro-2-iodo-1-(2-methoxyphenyl)-2-butenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 1 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

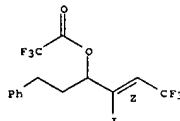
RN 908608-98-0 CAPLUS  
 CN 1-Naphthalenemethanol,  $\alpha$ -[(1Z)-3,3,3-trifluoro-1-iodo-1-propenyl]-, acetate (9CI) (CA INDEX NAME)

Double bond geometry as shown.



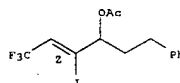
RN 908609-00-7 CAPLUS  
 CN Acetic acid, trifluoro-, (2Z)-4,4,4-trifluoro-2-iodo-1-(2-phenylethyl)-2-butenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 908609-01-8 CAPLUS  
 CN Benzenepropanol,  $\alpha$ -[(1Z)-3,3,3-trifluoro-1-iodo-1-propenyl]-, acetate (9CI) (CA INDEX NAME)

Double bond geometry as shown.

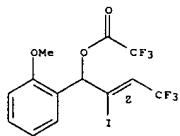


RN 908609-04-1 CAPLUS  
 CN Acetic acid, trifluoro-, 1-[(1Z)-3,3,3-trifluoro-1-iodo-1-propenyl]tridecyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

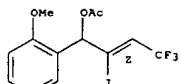


L4 ANSWER 1 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



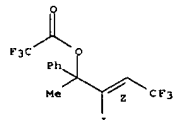
RN 908609-09-6 CAPLUS  
 CN Benzenemethanol, 2-methoxy- $\alpha$ -[(1Z)-3,3,3-trifluoro-1-iodo-1-propenyl]-, acetate (9CI) (CA INDEX NAME)

Double bond geometry as shown.



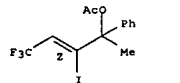
RN 908609-10-9 CAPLUS  
 CN Acetic acid, trifluoro-, (2Z)-4,4,4-trifluoro-2-iodo-1-methyl-1-phenyl-2-butenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 908609-11-0 CAPLUS  
 CN Benzenemethanol,  $\alpha$ -methyl- $\alpha$ -[(1Z)-3,3,3-trifluoro-1-iodo-1-propenyl]-, acetate (9CI) (CA INDEX NAME)

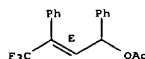
Double bond geometry as shown.



L4 ANSWER 1 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS  
 FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

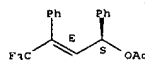
L4 ANSWER 2 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2006:283604 CAPLUS  
 DOCUMENT NUMBER: 144:488118  
 TITLE: Palladium-Catalyzed Regio- and Stereoselective  
 Formate  
 Reduction of Fluorine-Containing Allylic Mesylates. A New Entry for the Construction of a Tertiary Carbon Attached with a Fluoroalkyl Group  
 AUTHOR(S): Konno, Tsutomu; Takehana, Tsuyoshi; Mishima, Makoto; Ishihara, Takashi  
 CORPORATE SOURCE: Department of Chemistry and Materials Technology, Kyoto Institute of Technology, Kyoto, 606-8585, Japan  
 SOURCE: Journal of Organic Chemistry (2006), 71(9), 3545-3550  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 144:488118  
 AB The regioselective palladium-catalyzed formate reduction of  $\gamma$ -fluoroalkylated allylic esters is described. Reduction of the allylic esters under the influence of palladium with a monodentate phosphine ligand proceeded preferentially at the  $\gamma$  position, the corresponding reduction products with a fluoroalkyl group at the tertiary carbon being afforded in high yields. When the chiral allylic ester was employed, complete chirality transfer was observed, leading to the optically active materials in high yields.  
 IT 887616-49-1P 887616-75-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (palladium-catalyzed regio- and stereoselective formate reduction of  $\gamma$ -fluoroalkylated allylic esters)  
 RN 887616-49-1 CAPLUS  
 CN Benzenemethanol,  $\alpha$ -[(1E)-3,3,3-trifluoro-2-phenyl-1-propenyl]-, acetate (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 887616-75-3 CAPLUS  
 CN Benzenemethanol,  $\alpha$ -[(1E)-3,3,3-trifluoro-2-phenyl-1-propenyl]-, acetate, (uS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



L4 ANSWER 2 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS  
 FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 3 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2005:1330461 CAPLUS  
 DOCUMENT NUMBER: 144:69722  
 TITLE: Process for preparing 4-vinyl-2-oxo-1-pyrrolidine derivatives by intramolecular allylation  
 INVENTOR(S): Lurquin, Francoise; Driessens, Frank; Callaert, Michel  
 PATENT ASSIGNEE(S): Ucb, S.A., Belg.  
 SOURCE: PCT Int. Appl., 26 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005121082	A1	20051222	WO 2005-EP5689	20050526
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005251884	A1	20051222	AU 2005-251884	20050526
CA 2568700	A1	20051222	CA 2005-2568700	20050526
PRIORITY APPLN. INFO.:				
			EP 2004-13715	A 20040611
			WO 2005-EP5689	W 20050526

OTHER SOURCE(S): CASREACT 144:69722; MARPAT 144:69722  
 G1

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

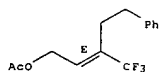
AB The present invention relates to a new process for preparing 2-oxo-1-pyrrolidine derivs. of general formula (I) [R2, R3 = H, C1-4 alkyl, cyano, aryl, -CO2R7, halogen, R8CO2, R9OSO2O or R11SO2O; R1 = Ra, Rb, C2-20 alkenyl, aryl-C2-20 alkenyl; X = CONR11R12, CO2R13, cyano, R7-R10 = H, Ra', Rb'; R11-R13 = H, C1-4 alkyl, aryl, arylalkyl, heteroaryl, heterocycloalkyl; Ra, Ra' = C1-20 alkyl or C1-20 alkyl substituted by one or more halogen, OH, SH, NH2, NO2, cyano, thiocyanato, CO2H, sulfonic acid, Rb, alkylsulfonyl, arylsulfonyl, alkylsulfinyl, arylsulfinyl, alkylthio, arylthio, alkoxy, aryloxy, sulfonamide, acyl, ester, amido, N3, acyloxy, esteroxy and/or amidoxy; Rb, Rb' = each (un)substituted aryl, heterocycloalkyl, or heteroaryl, comprising the cyclization of an intermediate of general formula (II) [R1-R3 = same as above; Y = a leaving group selected from halogen, -OC(O)R14, OSO2R15, etc.; R14, R15 = halogen, each (un)substituted alkyl, arylalkyl, or aryl; X1 is as defined for X; W = an electron withdrawing group selected from CO2R4, COMe, cyano, PO(OEt)2, SO2-aryl, -CO-aryl; R4 = H, each

L4 ANSWER 3 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
(un)substituted C1-6 alkyl, aryl, or arylalkyl in the presence of one or more org. and/or inorg. bases. Thus, a soln. of compd. (III) (304 g) in 607 mL MeCOEt was slowly added to a soln. of DBU (179 g) in 358 mL MeCOEt under stirring in a 2 L flask at room temp. for 1 h and treated with 300 mL 1 N HCl while keeping the temp. below 25° (pH = 6-7) to give, after workup, 384 g 4-(2,2-difluorovinyl)-2-oxopyrrolidine deriv. (IV) (R = Me) (99% yield). A soln. of 77.5 g Na2CO3 in 680 mL H2O was cooled to 20° and treated with a soln. of 85 g IV (R = Me) in MeOH and the resulting mixt. was stirred at 25° for 24 h. The aq. phase was extd. with iso-Pr acetate (2 X 170 mL), and then acidified with 121 mL concd. HCl to pH = 2 while maintaining the temp. below 25°. The mixt. was then stirred at room temp. for 20 h. The solid thus obtained was filtered, washed with H2O, and then dried under vacuum to give 55 g of crude acid IV (R = H) (68% yield) which was recrystd. from methanol to give pure compd. (V) (R5 = CO2H) as a white powder (70% yield). V (R5 = CO2H) (141.9 g) was suspended in 426 mL Me iso-Bu ketone and the suspension was heated at reflux for 6 h, cooled to room temp., concd. in vacuo to give, after recrystn. from Me iso-Bu ketone 71% V (R5 = H), namely (2S)-2-[(4S)-4-(2,2-difluorovinyl)-2-oxo-1-pyrrolidinyl]butanamide.  
IT 728040-39-9, Acetic acid 4,4,4-trifluoro-2-butenyl ester  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of 4-vinyl-2-oxo-1-pyrrolidine derivs. by intramol. allylation (cyclization) of N-(R-(leaving group)-substituted 2-butenyl)-α-(electron withdrawing group)-substituted acetamides)  
RN 728040-39-9 CAPLUS  
CN 2-Buten-1-ol, 4,4,4-trifluoro-, acetate (9CI) (CA INDEX NAME)

AcO-CH2-CH=CH-CF3

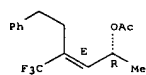
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
FORMAT

L4 ANSWER 4 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



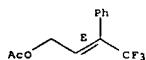
RN 821799-28-4 CAPLUS  
CN 3-Hexen-2-ol, 6-phenyl-4-(trifluoromethyl)-, acetate, (2R,3E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).  
Double bond geometry as shown.



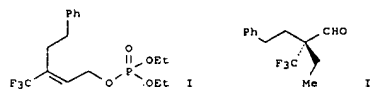
RN 821799-34-2 CAPLUS  
CN 2-Buten-1-ol, 4,4,4-trifluoro-3-phenyl-, acetate, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
FORMAT

L4 ANSWER 4 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2004:978761 CAPLUS  
DOCUMENT NUMBER: 142:113577  
TITLE: Construction of Optically Active CF3-Containing Quaternary Carbon Centers via Stereospecific SN2' Reaction  
AUTHOR(S): Kimura, Mitsuo; Yamazaki, Takashi; Kitezume, Tomoya; Kubota, Toshio  
CORPORATE SOURCE: Graduate School of Bioscience and Biotechnology, Tokyo  
Institute of Technology, Midori, Yokohama, 226-8501, Japan  
SOURCE: Organic Letters (2004), 6(25), 4651-4654  
CODEN: ORLEF7; ISSN: 1523-7060  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 142:113577  
GI



AB Phosphates,, e.g. I, from 3-substituted 4,4,4-trifluorobut-2-en-1-ols were found to be effective for construction of CF3-containing quaternary carbon centers by way of Cu(I)-catalyzed Grignard reactions in the presence of catalytic amts. of CuCN and trimethylsilyl chloride (TMSCl) in an anti SN2' manner. Addnl., this system can be readily extended to the chiral version with the aid of BINAL-H-mediated reduction, which, by way of ozonolysis of the reaction mixture obtained, eventually realized isolation of the optically active aldehyde II with the CF3-substituted quaternary carbon center.  
IT 821799-22-8P 821799-28-4P 821799-34-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(construction of optically active CF3-containing quaternary carbon centers via stereospecific SN2' reaction)  
RN 821799-22-8 CAPLUS  
CN 2-Penten-1-ol, 5-phenyl-3-(trifluoromethyl)-, acetate, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 5 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

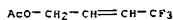
ACCESSION NUMBER: 2004:609970 CAPLUS  
DOCUMENT NUMBER: 141:158947  
TITLE: Allyl esters substituted by a perfluoromethylene group, their process of synthesis and their use, and a process for functionalizing a double bond  
INVENTOR(S): Roques, Nicolas  
PATENT ASSIGNEE(S): Rhodia Chimie, Fr.  
SOURCE: U.S. Pat. Appl. Publ., 21 pp., Cont.-in-part of U.S. Ser. No. 203,075.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 3  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004147789	A1	20040729	US 2003-740802	20031222
FR 2804955	A1	20010917	FR 2000-1744	20000211
FR 2804955	B1	20030214		
WO 2001058833	A1	20010816	WO 2001-FR364	20010212
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2003114721	A1	20030619	US 2002-203075	20020806
FR 2849025	A1	20040625	FR 2002-16308	20021220
FR 2849025	B1	20051014		
PRIORITY APPLN. INFO.:				
			FR 2000-1744	A 20000211
			WO 2001-FR364	W 20010212
			US 2002-203075	A2 20020806
			FR 2002-16308	A 20021220

OTHER SOURCE(S): MARPAT 141:158947  
AB This invention provides compds. RfRfC:CR3CH2O2, in which Rf is a radical that carries a perfluoromethylene group, which group ensures bonding to the remainder of the mol.: R1 and R3, which can be the same or different, are chosen from among hydrogen and alkyl or aryl radicals; X is an electroattractor group such that X-O-H is an acid whose pKa (in water) is at most equal to 8, advantageously 6, and preferably 5. These compds. are useful for the synthesis of nitrogen-containing heterocyclic compds.  
IT 728040-39-9P  
RL: IMP (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)  
(allyl esters substituted by a perfluoromethylene group, their process of synthesis and their use, and a process for functionalizing a double bond)  
RN 728040-39-9 CAPLUS



L4 ANSWER 5 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
CN 2-Buten-1-ol, 4,4,4-trifluoro-, acetate (9CI) (CA INDEX NAME)



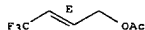
L4 ANSWER 6 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
R1R1CHCX2CH2OR3 (R1, R1-3 = same as in I, X = halo) with a strong N base of which the assocd. acid has pKa ≥12 or a N-free anionic base in polar solvents. Thus, contacting CF3CH2CHC1CH2OAc with 1 equiv. diazabicycloundecene 17 h at 0° in diisopropyl ether gave 83.22% CF3CH:CHCH2OAc.

IT 705977-03-3P, trans-4,4,4-Trifluoro-2-butenyl acetate  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of allyl esters substituted by difluoromethylene groups

by dehydrohalogenation for preparation nitrogen-containing heterocycles)

RN 705977-03-3 CAPLUS  
CN 2-Buten-1-ol, 4,4,4-trifluoro-, acetate, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE  
FORMAT

L4 ANSWER 6 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:515327 CAPLUS

DOCUMENT NUMBER: 141:53963

TITLE: Allyl esters substituted by a difluoromethylene group.

INVENTOR(S): their synthesis process, and their use  
Saint, James Laurent; Roques, Nicolas; Bernard, Jean Marie

PATENT ASSIGNEE(S): Rhodia Chimie, Fr.; Rhone Poulenc Chimie

SOURCE: Fr. Demande, 31 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2849025	A1	20040625	FR 2002-16308	20021220
FR 2849025	B1	20051014		
WO 2004065347	A1	20040805	WO 2003-FR3780	20031217
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003299334	A1	20040813	AU 2003-299334	20031217
EP 1631539	A1	20060308	EP 2003-799615	20031217
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, SK				
JP 2006511592	T	20060406	JP 2004-567023	20031217
US 2004147769	A1	20040729	US 2003-740802	20031222
US 2006069284	A1	20060330	US 2005-539639	20050616
PRIORITY APPLN. INFO.:				A 20000211
				WO 2001-FR364 W 20010212
				US 2002-203075 A2 20020806
				FR 2002-16308 A 20021220
				WO 2003-FR3780 W 20031217

OTHER SOURCE(S): MARPAT 141:53963

AB Trans-R1R1C:CR2CH2OR3 (R1 = group having a difluoromethylene group that bonds with the rest of the mol., R1, R2 = H, alkyl, or aryl, R3 = electron

attracting group such that ROH is an acid with pKa ≥8) (I), useful for preparation of N-containing heterocycles, are manufactured by contacting

L4 ANSWER 7 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:166411 CAPLUS

DOCUMENT NUMBER: 140:339049

TITLE: Trifluoromethylated vinylic and aromatic compounds from α-(trifluoromethyl)allyl alcohols

AUTHOR(S): Radix-Large, Sylvie; Kucharski, Stephanie; Langlois, Bernard R.

CORPORATE SOURCE: Laboratoire SERCOF (UMR 5181), Université Claude

Bernard-Lyon I, Villeurbanne, 69622, Fr.

SOURCE: Synthesis (2004), (3), 456-465

CODEN: SYNTBF; ISSN: 0039-7881

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:339049

AB α-(Trifluoromethyl)allyl alcs., easily available from α,β-unsatd. carbonyl compds., are readily converted into γ-(trifluoromethyl)allyl thioethers, benzyl ethers, trifluoroacetates, and azides. A Ph substituent at the γ-position to the hydroxyl function enhances their reactivity and the ease of SN2'

or

SN1' substitutions, whereas a Ph ring at the α-position allows the BF3-mediated synthesis of (trifluoromethyl)indenes. 4-Alkyl-4-methoxy-1-(trifluoromethyl)cyclohexa-2,5-dienols, readily available from 4-alkylphenols, are easily converted to 4-alkyl(trifluoromethyl)benzenes bearing a nucleophilic substituent (MeO, Cl) either on the ring or the benzylic position.

IT 681035-89-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

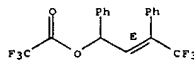
(preparation of trifluoromethylated vinylic and aromatic compds. from α-(trifluoromethyl)allyl alcs.)

RN 681035-89-2 CAPLUS

CN Acetic acid, trifluoro-, (2E)-4,4,4-trifluoro-1,3-diphenyl-2-butenyl

ester (9CI) (CA INDEX NAME)

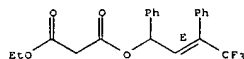
Double bond geometry as shown.



REFERENCE COUNT: 72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE  
FORMAT

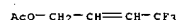
L4 ANSWER 8 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2004:153749 CAPLUS  
 DOCUMENT NUMBER: 140:374801  
 TITLE: Structure determination and molecular modelling of an unexpected side product of a cyclopropane lactone formation process  
 AUTHOR(S): Faigl, Ferenc; Finta, Zoltan; Hell, Zoltan; Karpati, Tamas; Harmat, Veronika; Koevesdi, Istvan; Toke, Laszlo  
 CORPORATE SOURCE: Research Group for Organic Chemical Technology, Budapest University of Technology and Economics, Hungarian Academy of Sciences, Budapest, H-1521, Hung.  
 SOURCE: Journal of Molecular Structure (2004), 691(1-3), 259-264  
 CODEN: JMOB4; ISSN: 0022-2860  
 PUBLISHER: Elsevier Science B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 140:374801  
 AB A new byproduct has been isolated from the reaction mixture of a single electron transfer induced one-pot synthesis of a cyclopropane derivative  
 Mol. structure of the new compound has been determined by spectroscopic and single crystal X-ray diffraction methods. Formation of this indenofuran derivative has been rationalized on the basis of mol. modeling calcns. at DFT level.  
 IT 283585-07-9  
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)  
 surface (cyclization; structure determination and potential modeling of an unexpected indenofuran byproduct of cyclopropane lactone formation)  
 RN 283585-07-9 CAPLUS  
 CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-1,3-diphenyl-2-butenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

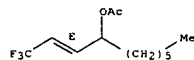
L4 ANSWER 9 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2004:28799 CAPLUS  
 DOCUMENT NUMBER: 141:227185  
 TITLE: Innovation at Rhodia Pharma Solutions. Part I - new trifluoromethylated aliphatic building blocks  
 AUTHOR(S): Roques, Nicolas; Galvez, Marie; Bonnefoy, Aude; Larquetoux, Laurent; Spagnol, Michel  
 CORPORATE SOURCE: Rhodia Pharma Solutions, Rhodia Inc, Cranbury, NJ, 08512-7500, USA  
 SOURCE: Chimica Oggi (2003), 21(9), 43-46  
 CODEN: CHOGDS; ISSN: 0392-839X  
 PUBLISHER: TeknoScienze  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 141:227185  
 AB A new concept in the field of direct trifluoromethylation strategies by successfully generating in situ the "naked" trifluoromethyl anion from potassium fluoroacetate decarboxylation or trifluoromethane deprotonation was introduced by Rhodia Pharma Solns. in 1995. This technol. led to the study of new industrial and economical route to potassium trifluoromethanesulfinate (CF<sub>3</sub>SO<sub>2</sub>K) and trifluoromethanesulfonyl chloride (CF<sub>3</sub>SO<sub>2</sub>Cl), which are key intermediates for the industrial production of triflic acid. The application of CF<sub>3</sub>SO<sub>2</sub>Cl as a reagent for the direct radical trifluoromethylation of simple terminal alkenes CH<sub>2</sub>=CHRR', such as vinyl, allyl or isoprenyl acetate, in order to synthesize CF<sub>3</sub>CH<sub>2</sub>CHC1RR' is discussed. Further basic chemical modifications of these primary precursors would lead to the production of final targeted building blocks CF<sub>3</sub>CH<sub>2</sub>-X, where X would be a reactive function (electrophile or nucleophile).  
 IT 728040-39-9P  
 RL: IMF (Industrial manufacture); PREP (Preparation) (manufacture of trifluoromethylated aliphatic building blocks via radical trifluoromethylation of terminal alkenes)  
 RN 728040-39-9 CAPLUS  
 CN 2-Buten-1-ol, 4,4,4-trifluoro-, acetate (9CI) (CA INDEX NAME)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

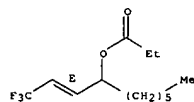
L4 ANSWER 10 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2002:151849 CAPLUS  
 DOCUMENT NUMBER: 136:340274  
 TITLE: Concise Syntheses of Nonracemic  $\gamma$ -Fluoroalkylated Allylic Alcohols and Amines Via an Enantiospecific Palladium-Catalyzed Allylic Substitution Reaction  
 AUTHOR(S): Konno, Tutomu; Nagata, Kensuke; Ishihara, Takashi; Yamanaka, Hiroki  
 CORPORATE SOURCE: Department of Chemistry and Materials Technology, Kyoto Institute of Technology, Sakyo-ku, Matsugasaki, Kyoto, 606-8585, Japan  
 SOURCE: Journal of Organic Chemistry (2002), 67(6), 1768-1775  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 136:340274  
 AB  $\alpha$ -Fluoroalkylated allyl mesylates reacted with various carboxylates and amines in the presence of tetrakis(triphenylphosphine)palladium(0) catalyst to give the corresponding  $\gamma$ -fluoroalkylated (E)-allylic alc. derivs. and amines, resp., in excellent yields. In almost all cases, no other regio- and stereoisomers were produced. Application of this palladium-catalyzed allylic substitution reaction to various nonracemic mesylates afforded chiral  $\gamma$ -fluoroalkylated allylic alc. derivs. and amines without any loss of enantiomeric excess through the reaction.  
 IT 320776-79-2P 320776-80-5P 320776-81-6P 320776-82-7P 320776-91-8P 320776-94-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of nonracemic  $\gamma$ -fluoroalkylated allylic alcs. and amines via enantiospecific palladium-catalyzed allylic substitution reaction)  
 RN 320776-79-2 CAPLUS  
 CN 2-Decen-4-ol, 1,1,1-trifluoro-, acetate, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 320776-80-5 CAPLUS  
 CN 2-Decen-4-ol, 1,1,1-trifluoro-, propanoate, (2E)- (9CI) (CA INDEX NAME)

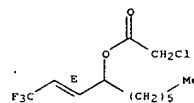
Double bond geometry as shown.



RN 320776-81-6 CAPLUS  
 CN Acetic acid, chloro-, 1-[(1E)-3,3,3-trifluoro-1-propenyl]heptyl ester (9CI) (CA INDEX NAME)

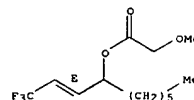
10539639a.trn

L4 ANSWER 10 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 Double bond geometry as shown.



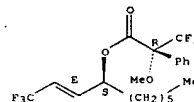
RN 320776-82-7 CAPLUS  
 CN Acetic acid, methoxy-, 1-[(1E)-3,3,3-trifluoro-1-propenyl]heptyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 320776-91-8 CAPLUS  
 CN Benzenecetic acid,  $\alpha$ -methoxy- $\alpha$ -(trifluoromethyl)-, (1S)-1-[(1E)-3,3,3-trifluoro-1-propenyl]heptyl ester, (4R)- (9CI) (CA INDEX NAME)

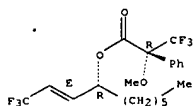
Absolute stereochemistry.  
 Double bond geometry as shown.



RN 320776-94-1 CAPLUS  
 CN Benzenecetic acid,  $\alpha$ -methoxy- $\alpha$ -(trifluoromethyl)-, (1R)-1-[(1E)-3,3,3-trifluoro-1-propenyl]heptyl ester, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.

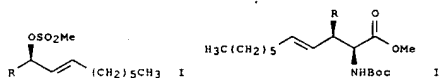
L4 ANSWER 10 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L4 ANSWER 11 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

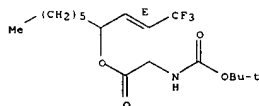
ACCESSION NUMBER: 2001:900021 CAPLUS  
DOCUMENT NUMBER: 136:325795  
TITLE: A novel and expedient synthesis of optically active fluoroalkylated amino acids via palladium-catalyzed allylic rearrangement and Ireland-Claisen rearrangement  
AUTHOR(S): Kenno, Tsutomu; Daitoh, Takeshi; Ishihara, Takashi; Yamanaka, Hiroki  
CORPORATE SOURCE: Department of Chemistry and Materials Technology, Kyoto Institute of Technology, Kyoto, Sakyo-ku, Matsugasaki, 606-8585, Japan  
SOURCE: Tetrahedron: Asymmetry (2001), 12(19), 2743-2748  
CODEN: TASYE3; ISSN: 0957-4166  
PUBLISHER: Elsevier Science Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 136:325795  
GI



AB The allylic substitution reactions of various chiral  $\alpha$ -fluoroalkylated mesylates with Boc-Gly-OH in the presence of a palladium catalyst proceeded smoothly to give  $\gamma$ -fluoroalkylated allyl esters in excellent yields. The esters were, then, directly subjected to Ireland-Claisen rearrangement, leading to the corresponding homochiral  $\alpha$ -fluoroalkylated- $\beta$ , $\gamma$ -unsatd. amino acids in good yields. For example, fluoroalkylated mesylates I (R = CF<sub>3</sub>, CHF<sub>2</sub>) reacted with Boc-Gly-OH in an one-pot allylic substitution, followed by Ireland-Claisen rearrangement and esterification with diazomethane to give amino acid esters II.  
IT 412948-88-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of optically active fluoroalkylated amino acids via palladium-catalyzed allylic substitution reaction and Ireland-Claisen rearrangement)  
RN 412948-88-0 CAPLUS  
CN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-, 1-[(1E)-3,3,3-trifluoro-1-propenyl]heptyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 11 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



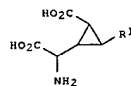
REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L4 ANSWER 12 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:881112 CAPLUS  
DOCUMENT NUMBER: 134:42439  
TITLE: Preparation of (carboxycyclopropyl)glycine derivatives  
INVENTOR(S): as excitatory amino acid receptor modulators  
Collado Cano, Ivan; Pedregal Tercero, Concepcion; Marcos Llorente, Alicia; Lopez de Uralde Garmendia, Beatriz; Gonzalez Garcia, Maria Rosario; Bueno Melendo, Ana Belen  
PATENT ASSIGNEE(S): Lilly, S.A., Spain  
SOURCE: PCT Int. Appl., 132 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000075101	A1	20001214	WO 2000-EP4903	20000526
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1189873	A1	20020327	EP 2000-935144	20000526
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 6498180	B1	20021224	US 2001-979322	20011116
PRIORITY APPLN. INFO.: EP 1999-500090 A 19990603				
WO 2000-EP4903 W 20000526				

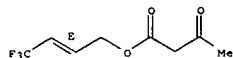
OTHER SOURCE(S): MARPAT 134:42439  
GI



AB (carboxycyclopropyl)glycine deriva. I [R1 is halo-C1-10 alkyl, halo-C2-10 alkenyl, or (CH2)nY in which n is 1 or 2 and Y is OH, CN, N3, OR3, SH, S(O)pR4, SO3H, NH2, NHR5, NR6R7, NHCOR8, NO2, CO2H, CONHR9, 1H-tetrazol-5-yl, 5-phenyltetrazol-2-yl, or PO3H2 (R3, R5, R6, R7, R8 and R9 are each selected independently from C1-4 alkyl, aryl and aryl-C1-4 alkyl; R4 is selected from C1-4 alkyl, aryl, aryl-C1-4 alkyl, 1H-tetrazol-5-yl, carboxy-C1-4 alkyl and 1H-tetrazol-5-yl-C1-4 alkyl; and p is 0-3)] or their salts or esters, provided that R1 is not

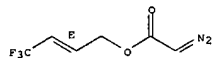
L4 ANSWER 12 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
methoxymethyl, modulate metabotropic glutamate receptor function and are useful in treating disorders of the central nervous system. Thus, (2SR,1'SR,2'RS,3'RS)-2-(3'-hydroxymethyl-2'-carboxycyclopropyl)glycine, prep'd. by a multistep procedure starting with reaction of cis-4,7-dihydro-1,3-dioxepin with Et diazoacetate, reversed [3H] LY341495 binding with a  $K_i$  of 66.1 nM at mGluR2 and 7.9 nM at mGluR3.  
IT 312912-67-7P 312912-68-8P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of (carboxycyclopropyl)glycine deriva. as excitatory amino acid receptor modulators)  
RN 312912-67-7 CAPLUS  
CN Butanoic acid, 3-oxo-, (2E)-4,4,4-trifluoro-2-butenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 312912-68-8 CAPLUS  
CN Acetic acid, diazo-, (2E)-4,4,4-trifluoro-2-butenyl ester (9CI) (CA INDEX NAME)

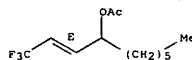
Double bond geometry as shown.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
FORMAT

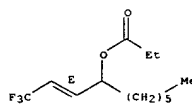
L4 ANSWER 13 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2000:845258 CAPLUS  
DOCUMENT NUMBER: 134:115669  
TITLE: Highly regio- and stereo-controlled Pd(0)-catalyzed nucleophilic substitution reaction for the synthesis of optically active  $\gamma$ -fluoroalkylated allylic alcohols  
AUTHOR(S): Konno, Tsutomu; Ishihara, Takashi; Yamanaka, Hiroki  
CORPORATE SOURCE: Department of Chemistry and Materials Technology, Kyoto Institute of Technology, Kyoto, 606-8585, Japan  
SOURCE: Tetrahedron Letters (2000), 41(44), 8467-8472  
CODEN: TELEAY; ISSN: 0040-4039  
PUBLISHER: Elsevier Science Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 134:115669  
AB Pd(0)-catalyzed nucleophilic substitution of optically active  $\alpha$ -(fluoroalkyl)allyl mesylates with various types of carboxylates proceeded regioselectively to afford the corresponding chiral  $\gamma$ -fluoroalkylated allylic alcs. in excellent yields without any loss of optical purities.  
IT 320776-79-2P 320776-80-5P 320776-81-6P 320776-82-7P 320776-91-8P 320776-94-1P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of  $\gamma$ -fluoroalkyl allyl alcs. by regio- and stereoselective palladium-catalyzed nucleophilic substitution)  
RN 320776-79-2 CAPLUS  
CN 2-Decen-4-ol, 1,1,1-trifluoro-, acetate, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 320776-80-5 CAPLUS  
CN 2-Decen-4-ol, 1,1,1-trifluoro-, propanoate, (2E)- (9CI) (CA INDEX NAME)

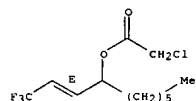
Double bond geometry as shown.



RN 320776-81-6 CAPLUS  
CN Acetic acid, chloro-, 1-[(1E)-3,3,3-trifluoro-1-propenyl]heptyl ester (9CI) (CA INDEX NAME)

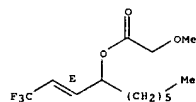
Double bond geometry as shown.

L4 ANSWER 13 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



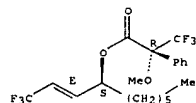
RN 320776-82-7 CAPLUS  
CN Acetic acid, methoxy-, 1-[(1E)-3,3,3-trifluoro-1-propenyl]heptyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



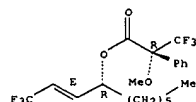
RN 320776-91-8 CAPLUS  
CN Benzenecetic acid,  $\alpha$ -methoxy- $\alpha$ -(trifluoromethyl)-, (1R)-1-[(1E)-3,3,3-trifluoro-1-propenyl]heptyl ester, (1R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



RN 320776-94-1 CAPLUS  
CN Benzenecetic acid,  $\alpha$ -methoxy- $\alpha$ -(trifluoromethyl)-, (1R)-1-[(1E)-3,3,3-trifluoro-1-propenyl]heptyl ester, (1R)- (9CI) (CA INDEX NAME)

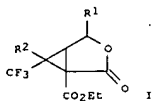
Absolute stereochemistry.  
Double bond geometry as shown.



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L4 ANSWER 14 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

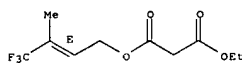
ACCESSION NUMBER: 2000:736571 CAPLUS  
 DOCUMENT NUMBER: 134:42035  
 TITLE: Stereoselective synthesis of trifluoromethylated cyclopropanecarboxylic acid derivatives  
 AUTHOR(S): Faigl, F.; Finta, Z.; Hell, Z.; Devenyi, T.; Kovacs, I.; Toke, L.  
 CORPORATE SOURCE: Szerviz Kemiai Technol. Tanszek, Budapesti Muszaki es Gazdasag-tudomanyi Egyetem, Budapest, 1521, Hung.  
 SOURCE: Magyar Kemiai Folyoirat (2000), 106(9), 341-346  
 CODEN: MGKFA3; ISSN: 0025-0155  
 PUBLISHER: Magyar Kemikusok Egyesulete  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Hungarian  
 OTHER SOURCE(S): CASREACT 134:42035  
 GI



AB Several new trifluoromethylated allylic alcs. and their monoethyl malonate esters were prepared. These esters underwent stereoselective and, in two cases stereospecific, cyclization reactions in the presence of iodine, potassium carbonate and a phase transfer catalyst to give title compds. I (R1 = H, Me, Ph; R2 = Me, Ph). The substituents (in the allyl and vinyl positions of the starting materials) influenced the diastereoselectivity of the SET induced multistep cyclization procedure.

IT 197566-48-6P 197566-49-7P 197566-50-OP  
 283584-99-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and stereoselective cyclization of)  
 RN 197566-48-6 CAPLUS  
 CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-3-methyl-2-butenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

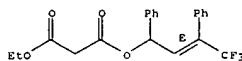


RN 197566-49-7 CAPLUS  
 CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-1,3-dimethyl-2-butenyl ester

L4 ANSWER 14 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

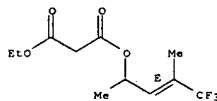
RN 283585-07-9 CAPLUS  
 CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-1,3-diphenyl-2-butenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



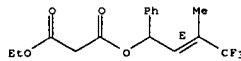
L4 ANSWER 14 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Double bond geometry as shown.



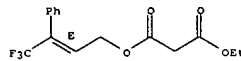
RN 197566-50-0 CAPLUS  
 CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-3-methyl-1-phenyl-2-butenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



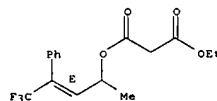
RN 283584-99-6 CAPLUS  
 CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-3-phenyl-2-butenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IT 283585-03-5P 283585-07-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and stereospecific cyclization of)  
 RN 283585-03-5 CAPLUS  
 CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-1-methyl-3-phenyl-2-butenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



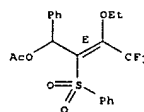
L4 ANSWER 15 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:643819 CAPLUS  
 DOCUMENT NUMBER: 133:335047  
 TITLE: First synthesis of an alpha-(trifluoromethyl)allenol ether via the Julia-Lythgoe process  
 AUTHOR(S): Yoshimatsu, Mitsuhiro; Hibino, Masaru  
 CORPORATE SOURCE: Department of Chemistry, Faculty of Education, Gifu University, Gifu, 501-1193, Japan  
 SOURCE: Chemical & Pharmaceutical Bulletin (2000), 48(9), 1395-1398  
 CODEN: CPBTAL; ISSN: 0009-2363  
 PUBLISHER: Pharmaceutical Society of Japan  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 133:335047

AB alpha-(Trifluoromethyl)allenol ethers were prepared in moderate to good yields by the Julia-Lythgoe process using beta-ethoxy-beta-(trifluoromethyl)vinyl Ph sulfone. Several reactions of 4-ClC6H4CH=C(CF3)OEt were examined to give alpha,beta-unsatd. trifluoromethyl ketone derivs.

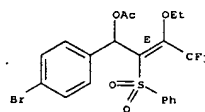
IT 303734-21-6P 303734-22-7P 303734-23-8P  
 303734-24-9P 303734-25-0P 303734-26-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (first synthesis of an alpha-(trifluoromethyl)allenol ether via Julia-Lythgoe process)  
 RN 303734-21-6 CAPLUS  
 CN Benzenemethanol, 4-bromo-alpha-[(1E)-2-ethoxy-3,3,3-trifluoro-1-(phenylsulfonyl)-1-propenyl]-, acetate (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 303734-22-7 CAPLUS  
 CN Benzenemethanol, 4-bromo-alpha-[(1E)-2-ethoxy-3,3,3-trifluoro-1-(phenylsulfonyl)-1-propenyl]-, acetate (9CI) (CA INDEX NAME)

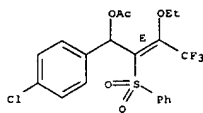
Double bond geometry as shown.



RN 303734-23-8 CAPLUS  
 CN Benzenemethanol, 4-chloro-alpha-[(1E)-2-ethoxy-3,3,3-trifluoro-1-

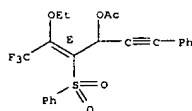
L4 ANSWER 15 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
(phenylsulfonyl)-1-propenyl)-, acetate (9CI) (CA INDEX NAME)

Double bond geometry as shown.



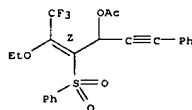
RN 303734-24-9 CAPLUS  
CN 4-Hexen-1-yn-3-ol, 5-ethoxy-6,6,6-trifluoro-1-phenyl-4-(phenylsulfonyl)-, acetate, (4E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 303734-25-0 CAPLUS  
CN 4-Hexen-1-yn-3-ol, 5-ethoxy-6,6,6-trifluoro-1-phenyl-4-(phenylsulfonyl)-, acetate, (4Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

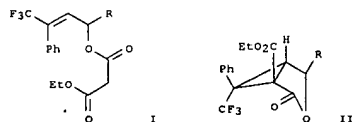


RN 303734-26-1 CAPLUS  
CN 1,4-Hexadien-3-ol, 5-ethoxy-6,6,6-trifluoro-1-phenyl-4-(phenylsulfonyl)-, acetate, (1E,4E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 16 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:168918 CAPLUS  
DOCUMENT NUMBER: 133:104927  
TITLE: Unexpected substituent effect in the stereoselective synthesis of trifluoromethyl group containing cyclopropane lactones  
AUTHOR(S): Faigl, F.; Finta, Z.; Hell, Z.; Kovacs, I.; Toké, L.  
CORPORATE SOURCE: Department of Organic Chemical Technology, Technical University of Budapest, Budapest, H-1521, Hung.  
SOURCE: Journal of Fluorine Chemistry (2000), 103(2), 117-121  
CODEN: JFLCAR; ISSN: 0022-1139  
PUBLISHER: Elsevier Science S.A.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 133:104927  
GI



AB Me or Ph substitution in the allylic position of malonic esters I (R = H, Me, Ph) of (E)-phenyl(trifluoromethyl)propenols resulted in unexpected and

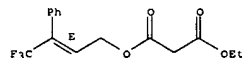
unprecedented stereospecific formation of the corresponding cyclopropane lactones II by a multistep reaction with iodine in the presence of potassium carbonate and phase transfer catalyst.

IT 283584-99-6P 283585-03-5P 283585-07-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reagent or reagent)

(substituent effect in stereoselective synthesis of trifluoromethyl cyclopropane lactones by cyclization of (trifluoromethyl)phenylpropenyl malonates)

RN 283584-99-6 CAPLUS  
CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-1-phenyl-2-butenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

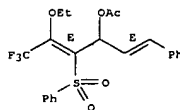


RN 283585-03-5 CAPLUS  
CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-1-methyl-3-phenyl-2-butenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

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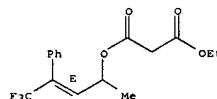
L4 ANSWER 15 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS

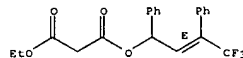
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L4 ANSWER 16 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 283585-07-9 CAPLUS  
CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-1,3-diphenyl-2-butenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS

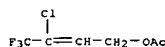
FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 17 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1999:736636 CAPLUS  
 DOCUMENT NUMBER: 131:352823  
 TITLE: Improved process for the preparation of trifluoromethyl containing derivatives  
 INVENTOR(S): Van Der Puy, Michael  
 PATENT ASSIGNEE(S): Alliedsignal Inc., USA  
 SOURCE: PCT Int. Appl., 16 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9958488	AI	19991118	WO 1999-US10438	19990513
WI: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG US 6111130 A 20000829 US 1999-307819 19990510 AU 9939852 A 19991129 AU 1999-39852 19990513 PRIORITY APPLN. INFO.: US 1998-85448P P 19980514 US 1999-307819 A 19990510 WO 1999-US10438 W 19990513				

OTHER SOURCE(S): MARPAT 131:352823  
 AB The present invention relates to a process for the preparation of trifluoromethylated derivs. of the formula CF<sub>3</sub>CCl:CHCH<sub>2</sub>O(R), wherein R is unsubstituted or substituted C1 to C6 straight chain or branched alkyl, unsubstituted or substituted C3 to C7 cycloalkyl, unsubstituted or substituted C2 to C12 alkenyl, a benzyl group unsubstituted or substituted with R', or a Ph group unsubstituted or substituted with R', wherein R' is an unsubstituted or substituted C1 to C6 straight chain or branched alkyl, and wherein where R and/or R' are substituted each is substituted with R', by reaction of CF<sub>3</sub>CCl<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Cl (HCFC-353) with carboxylic acid salts. The trifluoromethylated derivs., particularly CF<sub>3</sub>CCl:CHCH<sub>2</sub>O(C)CH<sub>3</sub>, are versatile intermediates for the synthesis of a wide variety of trifluoromethylated organic compds., which find utility as pharmaceuticals, agricultural chems., and materials such as liquid crystals. Thus, a mixture of sodium acetate (300 g), DMF (750 mL), and HCFC-353 (323 g) were heated

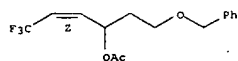
L4 ANSWER 17 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 to 70-75° for 40 h to give 76.6 g CF<sub>3</sub>CCl<sub>2</sub>CH:CH<sub>2</sub> and 173.0 g CF<sub>3</sub>CCl:CHCH<sub>2</sub>OAc. A mixt. of 90.4 g CF<sub>3</sub>CCl<sub>2</sub>CH:CH<sub>2</sub> and 3.0 g LiCl was heated to 95-105° for 3 h and reacted with 45 g sodium acetate at 80° for 1 h to give 86.1 g CF<sub>3</sub>CCl:CHCH<sub>2</sub>OAc with overall yield of CF<sub>3</sub>CCl:CHCH<sub>2</sub>OAc from HCFC-353 of 81%.  
 IT 216393-61-2P  
 RL: IMP (Industrial manufacture); PUR (Purification or recovery); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent) (optionally intermediate; preparation of trifluoromethyl containing derivs.)  
 RN 216393-61-2 CAPLUS  
 CN 2-Buten-1-ol, 3-chloro-4,4,4-trifluoro-, acetate (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

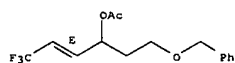
L4 ANSWER 18 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1999:533303 CAPLUS  
 DOCUMENT NUMBER: 131:322201  
 TITLE: CuCN and trimethylsilyl chloride-catalyzed regioselective Grignard reactions to CF<sub>3</sub>-containing allylic derivatives  
 AUTHOR(S): Yamazaki, Takashi; Umetani, Hideki; Kitazume, Tomoya  
 CORPORATE SOURCE: Department of Bioengineering, Tokyo Institute of Technology, Yokohama, 226-8501, Japan  
 SOURCE: Israel Journal of Chemistry (1999), 39(2), 193-205  
 CODEN: ISJCAT; ISSN: 0021-2148  
 PUBLISHER: Laser Pages Publishing  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 131:322201  
 AB CF<sub>3</sub>-containing allylic alc. derivs. were treated with an appropriate Grignard reagent in the presence of catalytic amts. of CuCN and trimethylsilyl chloride (TMSCl) to furnish products via the clean anti-SN<sub>2</sub>' mechanism. Exptl. results as well as ab initio computational analyses unambiguously demonstrated the important roles of TMSCl as a Lewis basic additive for smooth promotion of reductive elimination and inhibition of the "Cu<sub>2</sub>tpbond.F" elimination leading to undesired byproduct formation.  
 IT 197657-75-3 197657-84-4 197657-87-7  
 249283-58-7  
 RL: RCT (Reactant); RACT (Reactant or reagent) (copper cyanide and trimethylsilyl chloride-catalyzed regioselective Grignard reaction of (trifluoromethyl)allyl derivs.)  
 RN 197657-75-3 CAPLUS  
 CN 4-Hexen-3-ol, 6,6,6-trifluoro-1-(phenylmethoxy)-, acetate, (4E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 197657-84-4 CAPLUS  
 CN 4-Hexen-3-ol, 6,6,6-trifluoro-1-(phenylmethoxy)-, acetate, (4E)- (9CI) (CA INDEX NAME)

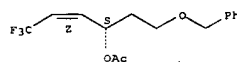
Double bond geometry as shown.



RN 197657-87-7 CAPLUS  
 CN 4-Hexen-3-ol, 6,6,6-trifluoro-1-(phenylmethoxy)-, acetate, (3S,4E)- (9CI) (CA INDEX NAME)

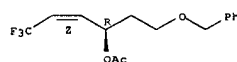
Absolute stereochemistry.  
 Double bond geometry as shown.

L4 ANSWER 18 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 249283-58-7 CAPLUS  
 CN 4-Hexen-3-ol, 6,6,6-trifluoro-1-(phenylmethoxy)-, acetate, (3R,4Z)- (9CI) (CA INDEX NAME)

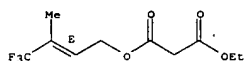
Absolute stereochemistry.  
 Double bond geometry as shown.



REFERENCE COUNT: 86 THERE ARE 86 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
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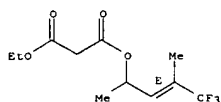
L4 ANSWER 19 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1997:635306 CAPLUS  
 DOCUMENT NUMBER: 127:318840  
 TITLE: Stereoselective synthesis of trifluoromethyl group containing cyclopropane lactones  
 AUTHOR(S): Faigl, Ferenc; Devenyi, Tamas; Lauko, Anna; Toke, Laszlo  
 CORPORATE SOURCE: Department of Organic Chemical Technology, Technical University of Budapest, Budapest, H-1521, Hung.  
 SOURCE: Tetrahedron (1997), 53(38), 13001-13008  
 CODEN: TETRAH; ISSN: 0040-4020  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 127:318840  
 AB Malonic acid esters of trans-1-substituted-3-trifluoromethyl-2-buten-1-ols underwent stereoselective, SET induced cyclization reaction sequence in the presence of iodine, potassium carbonate and quaternary ammonium salt. The allyl substituents of the starting materials influenced the diastereoisomeric composition of the new products.  
 IT 197566-48-6P 197566-49-7P 197566-50-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (stereoselective preparation of trifluoromethyl-substituted cyclopropane lactones)  
 RN 197566-48-6 CAPLUS  
 CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-3-methyl-2-butenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 197566-49-7 CAPLUS  
 CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-1,3-dimethyl-2-butenyl ester (9CI) (CA INDEX NAME)

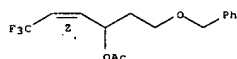
Double bond geometry as shown.



RN 197566-50-0 CAPLUS

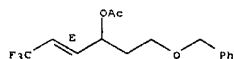
L4 ANSWER 20 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1997:626188 CAPLUS  
 DOCUMENT NUMBER: 127:318689  
 TITLE: Highly stereoselective SN2' reactions of Grignard reagents towards CF3-containing allylic acetates  
 AUTHOR(S): Yamazaki, Takashi; Umetani, Hideki; Kitazume, Tomoya  
 CORPORATE SOURCE: Dep. Bioeng., Tokyo Inst. Technol., Yokohama, 226, Japan  
 SOURCE: Tetrahedron Letters (1997), 38(38), 6705-6708  
 CODEN: TETLEA; ISSN: 0040-4039  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 127:318689  
 AB γ-Trifluoromethylated allylic acetates were found to quite smoothly proceed SN2' type reaction with various Grignard reagents in the presence of a catalytic amount of CuCN and TMS-Cl, without any trace amount of the corresponding SN2 products in all cases examined due to the electronic effect of a CF3 group.  
 IT 197657-75-3 197657-84-4  
 RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)  
 (stereoselective SN2' reactions of Grignard reagents towards CF3-containing allylic acetates)  
 RN 197657-75-3 CAPLUS  
 CN 4-Hexen-3-ol, 6,6,6-trifluoro-1-(phenylmethoxy)-, acetate, (4Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 197657-84-4 CAPLUS  
 CN 4-Hexen-3-ol, 6,6,6-trifluoro-1-(phenylmethoxy)-, acetate, (4E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



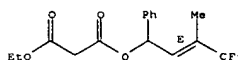
IT 197657-87-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (stereoselective SN2' reactions of Grignard reagents towards CF3-containing allylic acetates)  
 RN 197657-87-7 CAPLUS  
 CN 4-Hexen-3-ol, 6,6,6-trifluoro-1-(phenylmethoxy)-, acetate, (3S,4Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10539639a.trn

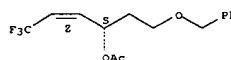
L4 ANSWER 19 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-3-methyl-1-phenyl-2-butenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L4 ANSWER 20 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 Double bond geometry as shown.



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT



L4 ANSWER 21 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1997:26204 CAPLUS  
 DOCUMENT NUMBER: 126:74346  
 TITLE: Highly Stereoselective Synthesis of Trifluoromethylated Compounds via Ester-Enolate [2,3]-Wittig and [3,3]-Ireland-Claissen Rearrangements  
 AUTHOR(S): Konno, Tsutomu; Umetani, Hideki; Kitazume, Tomoya  
 CORPORATE SOURCE: Department of Bioengineering, Tokyo Institute of Technology, Yokohama, 226, Japan  
 SOURCE: Journal of Organic Chemistry (1997), 62(1), 137-150  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB  $\gamma$ -Trifluoromethylated propargylic alcs. have been obtained in optically pure forms via effective enzymic kinetic resolution and then converted into (E)- or (Z)-allylic alcs. [2,3]-Wittig rearrangement of the corresponding [[ $\gamma$ -(trifluoromethyl)allyl]oxy]acetic acid Me esters afforded  $\alpha$ -hydroxy- $\beta$ -(trifluoromethyl)- $\gamma$ , $\delta$ -unsatd. carboxylic acid Me esters in good yields. The rearrangement of (Z)-substrates proceeded in a highly stereoselective manner to give anti-isomers with E configuration at a newly created olefinic bond via complete chirality transfer. (E)-Substrates, however, showed relatively low stereoselectivities resulting in mixts. of syn- and anti-products. The trifluoromethylated allylic alcs. were also converted into the corresponding  $\alpha$ -methoxyacetic acid  $\gamma$ -(trifluoromethyl)allyl esters and evaluated as substrates for [3,3]-Ireland-Claissen rearrangement. (E)-Substrates were efficiently transformed into syn-products while (Z)-substrates exhibited relatively low stereoselectivities. The two complementary methods provide facile routes to highly functionalized trifluoromethyl-containing mols. with a high

degree

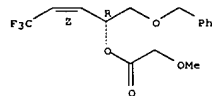
of stereocontrol.

IT 185424-05-9P 185424-06-0P 185424-07-1P  
 185424-08-2P 185424-09-3P 185424-10-6P  
 185424-11-7P 185424-12-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

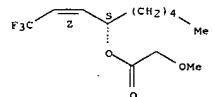
(stereoselective synthesis of trifluoromethylated compds. via ester-enolate [2,3]-Wittig and [3,3]-Ireland-Claissen rearrangements)

RN 185424-05-9 CAPLUS  
 CN Acetic acid, methoxy-, 4,4,4-trifluoro-1-[(phenylmethoxy)methyl]-2-butenyl ester, [R-(Z)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).  
 Double bond geometry as shown.

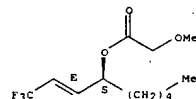


L4 ANSWER 21 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



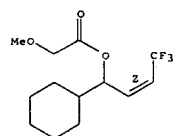
RN 185424-10-6 CAPLUS  
 CN Acetic acid, methoxy-, 1-(3,3,3-trifluoro-1-propenyl)hexyl ester, [S-(E)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).  
 Double bond geometry as shown.



RN 185424-11-7 CAPLUS  
 CN Acetic acid, methoxy-, 1-cyclohexyl-4,4,4-trifluoro-2-butenyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



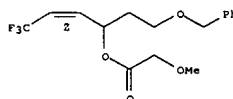
RN 185424-12-8 CAPLUS  
 CN Acetic acid, methoxy-, 1-cyclohexyl-4,4,4-trifluoro-2-butenyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 21 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

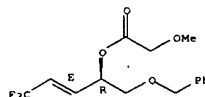
RN 185424-06-0 CAPLUS  
 CN Acetic acid, methoxy-, 4,4,4-trifluoro-1-[2-(phenylmethoxy)ethyl]-2-butenyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



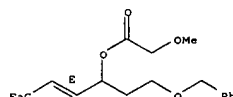
RN 185424-07-1 CAPLUS  
 CN Acetic acid, methoxy-, 4,4,4-trifluoro-1-[(phenylmethoxy)methyl]-2-butenyl ester, [R-(E)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).  
 Double bond geometry as shown.



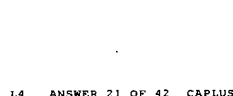
RN 185424-08-2 CAPLUS  
 CN Acetic acid, methoxy-, 4,4,4-trifluoro-1-[2-(phenylmethoxy)ethyl]-2-butenyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

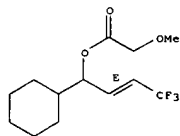


RN 185424-09-3 CAPLUS  
 CN Acetic acid, methoxy-, 1-(3,3,3-trifluoro-1-propenyl)hexyl ester, [S-(Z)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).  
 Double bond geometry as shown.



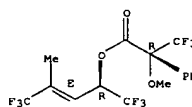
L4 ANSWER 21 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 22 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1996:693204 CAPLUS  
 DOCUMENT NUMBER: 126:103713  
 TITLE: Palladium(II)-catalyzed exchange and isomerization reactions. XVI The kinetics and stereochemistry of the oxidation and isomerization of hexafluoro allylic alcohols in aqueous solution catalyzed by PdCl<sub>3</sub>(pyridine)-  
 AUTHOR(S): Francis, John W.; Henry, Patrick M.  
 CORPORATE SOURCE: Department of Chemistry, Loyola University of Chicago,  
 SOURCE: Chicago, IL, 60626, USA  
 Journal of Molecular Catalysis A: Chemical (1996), 112(3), 317-326  
 CODEN: JMCCF2; ISSN: 1381-1169  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 126:103713  
 AB Further mechanistic studies on the PdCl<sub>3</sub>(pyridine)- catalytic system in aqueous solution are described using the tetrasubstituted allylic alc., (E)-2-methyl-d3-4-methyl-1,1,1,5,5,5-hexafluoro-3-penten-2-ol, 3a, and the trisubstituted allylic alc., (E)-4-Methyl-1,1,1,5,5,5-hexafluoro-3-penten-2-ol, 6, as substrates. At low [Cl-] the PdCl<sub>4</sub><sup>2-</sup> catalyzed isomerization of 3a, which can only undergo isomerization into its allylic isomer, was previously found to obey the Wacker rate expression:  $k_i[PdCl_4^{2-}][3a]/[H^+][Cl^-]^2$ . In contrast, the rate expression for isomerization of 3a by [PdCl<sub>3</sub>(Py)] at low [Cl-] was found to be:  $rate_i = k_i[PdCl_3(Py)][3a]/[Cl^-]$ . This rate expression is of the same form as that previously found for the isomerization of 3a by PdCl<sub>4</sub><sup>2-</sup> at high [Cl-]. This result strongly suggests that the hydroxypalladation by PdCl<sub>3</sub>(Py)- at low [Cl-] is a trans process as opposed to a cis process with PdCl<sub>4</sub><sup>2-</sup>. This expectation was confirmed by stereochem. studies with chiral 3a. The stereochem. of addition for PdCl<sub>3</sub>(Py)- was identical to that for PdCl<sub>4</sub><sup>2-</sup> at high [Cl-]. Independent stereochem. studies have shown this addition to be trans. With PdCl<sub>3</sub>(Py)- there are two possible routes for olefin oxidation. A cis process similar to that found for PdCl<sub>4</sub><sup>2-</sup> or a trans process analogous to that previously proposed to explain the trans stereochem. found at high [Cl-]. Stereochem. studies with 6, which can undergo oxidation, showed that both processes are operative with PdCl<sub>3</sub>(Py)- at [Cl-] = 0.05 M. Thus addition of a pyridine to the coordination sphere of Pd(II) causes a profound change in reactivity.  
 IT 185951-43-1P 185951-44-4P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (kinetics and stereochem. of oxidation and isomerization of aqueous hexafluoro allylic alcs. catalyzed by PdCl<sub>3</sub>(pyridine)-)

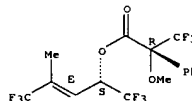
L4 ANSWER 22 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 RN 185951-43-3 CAPLUS  
 CN Benzeneacetic acid, α-methoxy-α-(trifluoromethyl)-, 4,4,4-trifluoro-3-methyl-1-(trifluoromethyl)-2-butenyl ester, [R-(R\*,R\*-(E))]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



RN 185951-44-4 CAPLUS  
 CN Benzeneacetic acid, α-methoxy-α-(trifluoromethyl)-, 4,4,4-trifluoro-3-methyl-1-(trifluoromethyl)-2-butenyl ester, [S-(R\*,S\*-(E))]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.

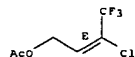


L4 ANSWER 23 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1996:661096 CAPLUS  
 DOCUMENT NUMBER: 125:300456  
 TITLE: Preparation of chlorotrifluorobutenes as synthetic intermediates  
 INVENTOR(S): Van Der Puy, Michael  
 PATENT ASSIGNEE(S): Alliedsignal Inc., USA  
 SOURCE: PCT Int. Appl., 16 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9628404	A1	19960919	WO 1996-US2963	19960301
W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, TJ, TM, TT, UA, UG, UZ, VN				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5654473	A	19970805	US 1995-405312	19950316
AU 9651357	A	19961002	AU 1996-51357	19960301
EP 815066	A1	19980107	EP 1996-507923	19960301
EP 815066	B1	20000105		
R: ES, FR, GB, IT				
JP 11501922	T	19990216	JP 1996-527678	19960301
TW 393451	B	20000611	TW 1996-85103382	19960321
PRIORITY APPLN. INFO.:			US 1995-405312	A 19950316
			WO 1996-US2963	W 19960301

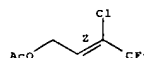
OTHER SOURCE(S): MARPAT 125:300456  
 AB CF3CCl=CHCH2R (R = H, F, Br, iodo, OAc) were prepared. Thus, CF3CCl<sub>3</sub> was added to CH<sub>2</sub>:CH<sub>2</sub> and the product treated with Cr<sub>2</sub>O<sub>3</sub> to give CF3CCl:CHCH<sub>2</sub>Cl which was treated with KOAc to give CF3CCl:CHCH<sub>2</sub>OAc.  
 IT 175401-09-9P 175401-10-2P  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of chlorotrifluorobutenes as synthetic intermediates)  
 RN 175401-09-9 CAPLUS  
 CN 2-Buten-1-ol, 3-chloro-4,4,4-trifluoro-, acetate, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



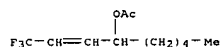
RN 175401-10-2 CAPLUS  
 CN 2-Buten-1-ol, 3-chloro-4,4,4-trifluoro-, acetate, (Z)- (9CI) (CA INDEX NAME)

L4 ANSWER 23 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 Double bond geometry as shown.



## L4 ANSWER 24 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

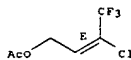
ACCESSION NUMBER: 1996:271988 CAPLUS  
 DOCUMENT NUMBER: 125:57876  
 TITLE: Stereochemical control in the silyl triflate-mediated Claisen rearrangement of allylic esters  
 AUTHOR(S): Kobayashi, Masatada; Masumoto, Katsuhisa; Nakai, Ei-ichi; Nakai, Takeshi  
 CORPORATE SOURCE: Dep. Chem. Technol., Tokyo Inst. Technol., Tokyo, Japan  
 SOURCE: Tetrahedron Letters (1996), 37(17), 3005-8  
 CODEN: TELEYA; ISSN: 0040-4039  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 125:57876  
 AB The titled Claisen modification proceeded with a remarkably high level of diastereoselection and asym. transmission by virtue of the proper choice of the combination of the silyl triflate and the tertiary amine used.  
 IT 178251-42-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (stereochem. control in the silyl triflate-mediated Claisen rearrangement of allylic esters)  
 RN 178251-42-8 CAPLUS  
 CN 2-Nonen-4-ol, 1,1,1-trifluoro-, acetate (9CI) (CA INDEX NAME)



## L4 ANSWER 25 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

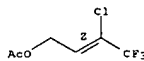
ACCESSION NUMBER: 1996:106832 CAPLUS  
 DOCUMENT NUMBER: 124:260321  
 TITLE: Preparation, fluorination and synthetic utility of a CFC-olefin adduct  
 AUTHOR(S): Van der Puy, Michael; Demmin, Timothy R.; Bindu Madhavan, G. V.; Thenappan, Alagappan; Tung, Harry S.  
 CORPORATE SOURCE: AlliedSignal Inc., Buffalo Research Laboratory, 20 Peabody Street, Buffalo, NY, 14210, USA  
 SOURCE: Journal of Fluorine Chemistry (1996), 76(1), 49-54  
 CODEN: JFLCAR; ISSN: 0022-1139  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 124:260321  
 AB 1,1,1-Trichlorotrifluoroethane was added to ethylene using the catalyst system  $\text{Fe}(\text{triethyl phosphite})_3$ , which eliminated the need for a solvent and avoided the corrosion problems inherent in  $\text{CuCl}$ -catalyzed reactions. The adduct,  $\text{CF}_3\text{CCl}_2\text{CH}_2\text{CH}_2\text{Cl}$ , was fluorinated with HF over a chromium(III) oxide catalyst. A series of alternating dehydrochlorinations and HF addns. to internal C:C double bonds was proposed and supported by thermodyn. calcns. to explain the formation of  $\text{CF}_3\text{CF}_2\text{CH}=\text{CH}_2$  as the principal fluorination product. An intermediate,  $\text{CF}_3\text{CCl}:\text{CHCH}_2\text{Cl}$ , formed cleanly by dehydrochlorination of the adduct in the absence of HF, was converted into 4,4,4-trifluorobutanol and other compds. of the type  $\text{CF}_3\text{CCl}:\text{CHCH}_2\text{X}$  (X = OAc, OH, Br, I, R).  
 IT 175401-09-9P 175401-10-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation, fluorination, and synthetic utility of a CFC-olefin adduct)  
 RN 175401-09-9 CAPLUS  
 CN 2-Buten-1-ol, 3-chloro-4,4,4-trifluoro-, acetate, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



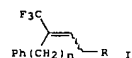
RN 175401-10-2 CAPLUS  
 CN 2-Buten-1-ol, 3-chloro-4,4,4-trifluoro-, acetate, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

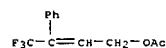


## L4 ANSWER 26 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:298199 CAPLUS  
 DOCUMENT NUMBER: 120:298199  
 TITLE: Synthesis of  $\gamma$ -trifluoromethylated primary allylic amines  
 AUTHOR(S): Felix, Caroline; Laurent, Andre; Lebideau, Frank; Mison, Pierre  
 CORPORATE SOURCE: Lab. Chim. Org., Univ. Claude Bernard-Lyon 1, Villeurbanne, 69622, Fr.  
 SOURCE: Journal of Chemical Research, Synopses (1993), (10), 389  
 CODEN: JRPSCD; ISSN: 0308-2342  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 120:298199  
 GI

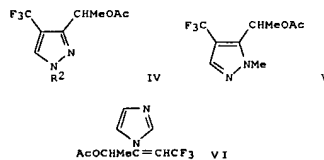


AB Preparation of trifluoromethylated primary allylic amines, e.g.,  $\text{Ph}(\text{CH}_2)_n\text{C}(\text{CF}_3)=\text{CHCH}_2\text{NH}_2$  was achieved starting from alcs.,  $\text{Ph}(\text{CH}_2)_n\text{C}(\text{CF}_3)(\text{OH})\text{CH}_2\text{CH}_2$  (1, n = 0, 1, 2). 1 was converted to the azide derivative 1 (R = N3) by mesylation with mesyl chloride in  $\text{CH}_2\text{Cl}_2$  followed by treatment with  $\text{NaN}_3$  in DMF. Reduction of azide 1 (R = N3) by  $\text{PPh}_3/\text{H}_2\text{O}$  gave allylic amine 1 (R = NH2) as mixts. of E and Z isomers. Allylic amines 1 (R = NH2) were converted to amides 1 (R =  $\text{NHCOPh}$ ) by  $\text{NEt}_3\text{-PhCOCl}$  in  $\text{CH}_2\text{Cl}_2$ .  
 IT 154841-07-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 154841-07-3 CAPLUS  
 CN 2-Buten-1-ol, 4,4,4-trifluoro-3-phenyl-, acetate (9CI) (CA INDEX NAME)



## L4 ANSWER 27 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

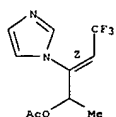
ACCESSION NUMBER: 1993:560183 CAPLUS  
 DOCUMENT NUMBER: 119:160183  
 TITLE: Fluorinated acetylenes. Part 8. Preparation and some reactions of 5,5,5-trifluoropent-3-yn-2-ol and the 5,5,5-trifluoro-1-phenylpent-3-yn-2-ol and the ester, 2-acetoxy-5,5,5-trifluoropent-3-yn-2-ol  
 AUTHOR(S): Sibous, Lakhdar; Tipping, Anthony E.  
 CORPORATE SOURCE: Chem. Dep., Univ. Manchester Inst. Sci. Technol., Manchester, M60 1QD, UK  
 SOURCE: Journal of Fluorine Chemistry (1993), 62(1), 39-49  
 CODEN: JFLCAR; ISSN: 0022-1139  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 119:160183  
 GI



AB Treatment of  $\text{CF}_3\text{C}(\text{tBu})\text{C}\equiv\text{C}\text{Li}$  with the aldehydes  $\text{RCH}_2\text{CHO}$  (R = H and Ph) affords the secondary alcs.  $\text{CF}_3\text{C}(\text{tBu})\text{C}\equiv\text{CCH}_2\text{OR}$  [R = Me (I) and R =  $\text{CH}_2\text{Ph}$  (II)]. Alc. I does not give the corresponding ketone on attempted oxidation (pyridinium chlorochromate or  $\text{Na}_2\text{Cr}_2\text{O}_7/\text{H}_2\text{SO}_4$ ), but alc. II is oxidized to the diketone  $\text{CF}_3\text{C}(\text{tBu})\text{C}\equiv\text{C}(\text{COCH}_2\text{Ph})_2$  (41%).  
 by active  $\text{MnO}_2$ . The acetate  $\text{CF}_3\text{C}(\text{tBu})\text{C}\equiv\text{CCH}_2\text{OAc}$  (III) undergoes facile reaction with diazomethane to give [(acetoxy)ethyl(trifluoromethyl)pyrazol  
 e IV (R2 = H) and hence [(acetoxy)ethyl]methyl(trifluoromethyl)pyrazoles IV (R2 = Me) and V, resp. Cycloaddn. also takes place between III and furan, but the major products (considered to be isomeric 1:1 adducts) have not been fully characterized. Although, III undergoes reaction with trifluoronitrosomethane, a cycloadduct has not been isolated, while nucleophilic attack by imidazole on the triple bond leads to the (Z)-alkene VI.  
 IT 149978-99-4P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 149978-99-4 CAPLUS  
 CN 1H-Imidazole-1-ethanol,  $\alpha$ -methyl- $\beta$ -(2,2,2-trifluoroethylidene)-, acetate (ester), (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 27 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 28 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1992:489692 CAPLUS

DOCUMENT NUMBER: 117:89692

TITLE: Palladium(II)-catalyzed exchange and isomerization reactions. 15. Kinetics and stereochemistry of the isomerization of 2-(methyl-d3)-4-methyl-1,1,1,5,5,5-hexafluoro-3-penten-2-ol in aqueous solution

catalyzed by PdCl<sub>4</sub><sup>2-</sup> at high chloride concentrations

AUTHOR(S): Francis, John W.; Henry, Patrick M.  
CORPORATE SOURCE: Dep. Chem., Loyola Univ., Chicago, IL, 60626, USA  
SOURCE: Organometallics (1992), 11(8), 2832-6

CODEN: ORGND7; ISSN: 0276-7333

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The isomerization of 2-(methyl-d3)-4-methyl-1,1,1,5,5,5-hexafluoro-3-penten-2-ol (2a) into an equilibrium mixture of 2a and

2-methyl-4-(methyl-d3)-

1,1,1,5,5,5-hexafluoro-3-penten-2-ol (2b) in aqueous solution was studied by 1H

and 2H NMR spectroscopy under conditions of high chloride (>2.0 M) concentration

used previously in the presence of CuCl<sub>2</sub> to determine the stereochem. of hydroxypalladation. The rate expression under these conditions is rate = k<sub>1</sub>[PdCl<sub>4</sub><sup>2-</sup>][2a]/[Cl<sup>-</sup>], with k<sub>1</sub> = 1.1 × 10<sup>-3</sup> s<sup>-1</sup>. This rate expression at high chloride concns. is identical to the rate expression found for the nonoxidative isomerization of allyl alc. under the same reaction conditions and is consistent with an equilibrium π-complex formation followed by trans attack of water to give the oxypalladation

intermediate, which reverses the process to give exchange. The fact that the attack is from outside the coordination sphere of the palladium(II) explains the single-chloride inhibition. Stereochem. studies were conducted with chiral (E)-2a. The observed result was the formation of chiral 2b with the

same configuration as the initial 2a but with the 2 geometric configuration. This result is also consistent only with trans hydroxypalladation. The result also agrees with earlier stereochem. studies at high chloride concns. which used quite a different technique. The important point is that since the exchange stereochem. studies

carried out in the previous paper of this series showed the hydroxypalladation to have stereochem. opposite from that at high chloride concns., the previous

stereochem. studies at high [Cl<sup>-</sup>] are not a valid indication of the stereochem. at low [Cl<sup>-</sup>].

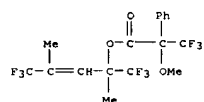
IT 142484-36-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and resolution of)

RN 142484-36-4 CAPLUS

CN Benzeneacetic acid, α-methoxy-α-(trifluoromethyl)-, 4,4,4-trifluoro-1,3-dimethyl-1-(trifluoromethyl)-2-butenyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 28 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



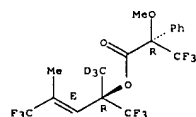
IT 135708-35-9P 142508-62-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 135708-35-9 CAPLUS

CN Benzeneacetic acid, α-methoxy-α-(trifluoromethyl)-, 4,4,4-trifluoro-3-methyl-1-(methyl-d3)-1-(trifluoromethyl)-2-butenyl ester, [R-[R',R'-(E)]]- (9CI) (CA INDEX NAME)

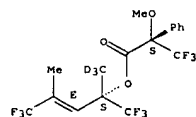
Absolute stereochemistry.  
Double bond geometry as shown.



RN 142508-62-1 CAPLUS

CN Benzeneacetic acid, α-methoxy-α-(trifluoromethyl)-, 4,4,4-trifluoro-3-methyl-1-(methyl-d3)-1-(trifluoromethyl)-2-butenyl ester, [S-[R',R'-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



L4 ANSWER 29 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1991:632522 CAPLUS

DOCUMENT NUMBER: 115:232522

TITLE: Synthesis of cis-configured bis(trifluoromethyl)pyrethroids

AUTHOR(S): Rothermel, Reinfried; Hanack, Michael  
CORPORATE SOURCE: Inst. Org. Chem., Univ. Tuebingen, Tuebingen, D-7400, Germany  
SOURCE: Liebigs Annalen der Chemie (1991), (10), 1013-20

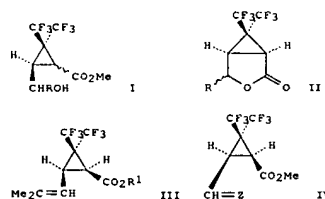
CODEN: LACHDL; ISSN: 0170-2041

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 115:232522

GI



AB trans-2,2-Bis(trifluoromethyl)cyclopropanecarboxylates I (R = Me<sub>2</sub>CH, H) are converted into the cis-diastereomers by base-catalyzed epimerization via the bicyclic lactones II. Dehydration of cis-I (R = Me<sub>2</sub>CH, H) and cleavage of the ester function leads to the fluorinated chrysanthemic

acid III (R = H), which is converted into the pyrethroids III (R = CH<sub>2</sub>CH<sub>2</sub>OPh-3, CH(CN)CH<sub>2</sub>OPh-3). cis-I (R = H) is oxidized by pyridinium chlorochromate to give Me

cis-3-formyl-2,2-bis(trifluoromethyl)cyclopropanecarboxylate (hexafluorocoronaraldehydic acid Me ester; IV; Z = O). This compound, which is very sensitive to isomerization, is converted into the pyrethroid esters IV [Z = C(CF<sub>3</sub>)<sub>2</sub>CH<sub>2</sub>] predominantly retaining the cis configuration; however, by introducing the 2,2-dichlorovinyl side chain the trans diastereomer is obtained. The starting materials trans-I are prepared by the reaction of aldehydes AcOCHR<sub>2</sub>CHO (R<sub>2</sub> = Me<sub>2</sub>CH, H) with CF<sub>3</sub>CCl<sub>2</sub>CF<sub>3</sub> and PPh<sub>3</sub> followed by cyclopropanation of the resulting 1,1-bis(trifluoromethyl)olefins, AcOCHR<sub>2</sub>CH: C(CF<sub>3</sub>)<sub>2</sub>, with (ethoxycarbonylmethylene)dimethylsulfurane, Me<sub>2</sub>S:CHCO<sub>2</sub>Et.

IT 121618-14-2P

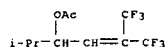
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclopropanation of, with (ethoxycarbonylmethylene)dimethyl sulfurane)

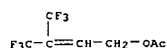
RN 121618-14-2 CAPLUS

CN 4-Hexen-3-ol, 6,6,6-trifluoro-2-methyl-5-(trifluoromethyl)-, acetate (9CI)

L4 ANSWER 29 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
(CA INDEX NAME)



IT 135524-49-1P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)  
RN 135524-49-1 CAPLUS  
CN 2-Buten-1-ol, 4,4,4-trifluoro-3-(trifluoromethyl)-, acetate (9CI) (CA INDEX NAME)



L4 ANSWER 30 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1991:582350 CAPLUS

DOCUMENT NUMBER: 115:182350

TITLE: Palladium(II)-catalyzed exchange and isomerization reactions. 14. Kinetics and stereochemistry of the isomerization and water exchange of

2-(methyl-d3)-4-methyl-1,1,1,5,5,5-hexafluoro-3-penten-2-ol in aqueous solution catalyzed by PdCl4<sup>2-</sup>. Two new mechanistic probes for catalytic chemistry Francis, John W.; Henry, Patrick M. Dep. Chem., Loyola Univ. Chicago, Chicago, IL, 60626, USA

SOURCE: Organometallics (1991), 10(10), 3498-503  
CODEN: ORGN7; ISSN: 0276-7333

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The isomerization of 2-(methyl-d3)-4-methyl-1,1,1,5,5,5-hexafluoro-3-penten-2-ol (I) into an equilibrium mixture of I and 2-methyl-4-(methyl-d3)-

1,1,1,5,5,5-hexafluoro-3-penten-2-ol (II) in aqueous solution was studied by 1H

and 2H NMR, under the Wacker conditions of low chloride (<1.0M) and acid (<0.5M) concns. The rate expression under these conditions was determined. The

exchange of I with 18O-enriched water was studied by 13C NMR using isotope-induced shift methods and the rate of exchange was found to be the

same as the rate of isomerization within exptl. error. This result requires that isomerization and exchange occur by a hydroxypalladation route, rather than through palladium(IV)-π-allyl intermediates. The rate expression for isomerization at low chloride concns. is identical with the rate expression for the Wacker oxidation of ethene to acetaldehyde.

This result is inconsistent with a proton inhibition arising from equilibrium

hydroxypalladation but is consistent with proton loss from the Pd(II) coordination sphere in a preequil. step followed by a cis hydroxypalladation occurring from within the coordination sphere of the palladium(II). Stereochem. studies were conducted with chiral (E)-1. The observed result was the formation of chiral 11 with the opposite configuration of the initial 1. This result is also consistent only with cis hydroxypalladation; so both kinetic and stereochem. mechanistic probes

give the same result.

IT 135708-35-9P 135708-36-OP 135708-37-1P  
135708-38-2P

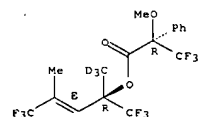
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 135708-35-9 CAPLUS

CN Benzeneacetic acid, α-methoxy-α-(trifluoromethyl)-, 4,4,4-trifluoro-3-methyl-1-(methyl-d3)-1-(trifluoromethyl)-2-butenyl ester, [R-[R\*,R\*-(E)]]- (9CI) (CA INDEX NAME)

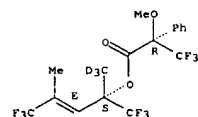
Absolute stereochemistry.  
Double bond geometry as shown.

L4 ANSWER 30 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



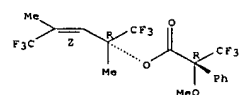
RN 135708-36-0 CAPLUS  
CN Benzeneacetic acid, α-methoxy-α-(trifluoromethyl)-, 4,4,4-trifluoro-3-methyl-1-(methyl-d3)-1-(trifluoromethyl)-2-butenyl ester, [S-[R\*,R\*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



RN 135708-37-1 CAPLUS  
CN Benzeneacetic acid, α-methoxy-α-(trifluoromethyl)-, 4,4,4-trifluoro-1,3-dimethyl-1-(trifluoromethyl)-2-butenyl ester, [R-[R\*,R\*-(Z)]]- (9CI) (CA INDEX NAME)

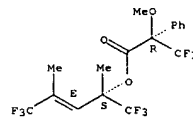
Absolute stereochemistry.  
Double bond geometry as shown.



RN 135708-38-2 CAPLUS  
CN Benzeneacetic acid, α-methoxy-α-(trifluoromethyl)-, 4,4,4-trifluoro-1,3-dimethyl-1-(trifluoromethyl)-2-butenyl ester, [S-[R\*,R\*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.

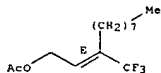
L4 ANSWER 30 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 31 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

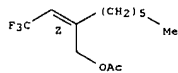
ACCESSION NUMBER: 1990:514701 CAPLUS  
 DOCUMENT NUMBER: 113:114701  
 TITLE: Trifluoromethylated allylic anion and radical;  
 generation by the electronic inversion of  $\pi$ -allylic  
 palladium complex by samarium diiodide  
 AUTHOR(S): Hanzawa, Yuji; Ishizawa, Seiji; Kobayashi, Yoshiro;  
 Taguchi, Takeo  
 CORPORATE SOURCE: Tokyo Coll. Pharm., Hachioji, 192-03, Japan  
 SOURCE: Chemical & Pharmaceutical Bulletin (1990), 38(4),  
 1104-6  
 CODEN: CPBTAL; ISSN: 0009-2363  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 113:114701  
 AB Trifluoromethylated  $\pi$ -allylic Pd complexes were treated with SmI2 to  
 generate the trifluoromethylated allylic anion and radical species, which  
 undergo reduction, elimination, or dimerization reactions. Treatment of  
 PhCH2CH2CH(OAc)C(CF3):CH2 with Pd(PPh3)4 and SmI2 in the presence of  
 MeCO(CH2)5Me gave 76% of a 4:3 isomeric mixture of adducts  
 PhCH2CH2CH(CF3):CH2CMe(OH)(CH2)5Me.  
 IT 120596-31-8 120596-33-0 129049-09-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with palladium tetrakis(triphenylphosphine) and samarium  
 diiodide, allylic anion and radical species from)  
 RN 120596-31-8 CAPLUS  
 CN 2-Undecen-1-ol, 3-(trifluoromethyl)-, acetate, (E)- (9CI) (CA INDEX  
 NAME)

Double bond geometry as shown.



RN 120596-33-0 CAPLUS  
 CN 1-Octanol, 2-(2,2,2-trifluoroethylidene)-, acetate, (Z)- (9CI) (CA INDEX  
 NAME)

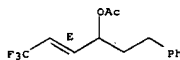
Double bond geometry as shown.



RN 129049-09-8 CAPLUS  
 CN Benzenepropanol,  $\alpha$ -(3,3,3-trifluoro-1-propenyl)-, acetate, (E)-  
 (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 31 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 32 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1990:497086 CAPLUS  
 DOCUMENT NUMBER: 113:97086  
 TITLE: Preparation of optically active  
 trifluoromethylhydroxycyclopropanes  
 INVENTOR(S): Kitatsune, Tomoya; Takeda, Mitsunori  
 PATENT ASSIGNEE(S): Kashima Oil Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02049742	A	19900220	JP 1988-200229	19880812
JP 2642959	B2	19970820		
PRIORITY APPLN. INFO.:			JP 1988-200229	19880812

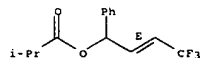
OTHER SOURCE(S): MARPAT 113:97086

GI



AB The title compds. (I: R1, R2 = C1-2 fluoroalkyl, C1-10 alkyl, C7-10  
 aralkyl, C6-10 aryl; provided that 2l of R1, R2 = C1-2 fluoroalkyl)  
 of high optical purity, useful as intermediates for enzyme inhibitors,  
 physiol. active substances, antitumor agents, and ferroelec. liquid  
 crystals, were prepared. Thus, reduction of CF3CH(OH)C.tplbond.CPh with  
 Na[AlH2COCH2CH2OMe]2 in Et2O followed by acetylation with AcCl in  
 pyridine gave CF3CH(OAc)CH:CHPh. Stereoselective hydrolysis of the  
 latter  
 with lipase MY in H2O at 40-41° for 6.5 h gave (3S)-(E)-  
 CF3CH(OR3)CH:CHPh (R3 = Ac) and (3R)-(E)-CF3CH(OR3)CH:CHPh (R3 = H) (II).  
 Carbene addition reaction of II with CH2I2 in the presence of Sm and  
 HgCl2 in  
 THF at 0° for 1 h and room temperature for 2 h gave (1R)-(+)-I (R1 = CF3,  
 R2 = Ph).  
 IT 128726-32-9p  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and carbene addition of, with methylene iodide)  
 RN 128726-32-9 CAPLUS  
 CN Propanoic acid, 2-methyl-, 4,4,4-trifluoro-1-phenyl-2-butenyl ester, (E)-  
 (9CI) (CA INDEX NAME)

Double bond geometry as shown.

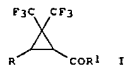


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L4 ANSWER 32 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSWER 33 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

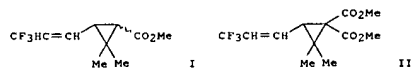
ACCESSION NUMBER: 1989:554137 CAPLUS  
 DOCUMENT NUMBER: 111:154137  
 TITLE: Synthesis of bis(trifluoromethyl) substituted pyrethroids  
 AUTHOR(S): Mack, Helmut; Hanack, Michael  
 CORPORATE SOURCE: Inst. Organische Chemie, Universitat Tübingen, Tübingen, D-7400, Fed. Rep. Ger.  
 SOURCE: Liebigs Annalen der Chemie (1989), (9), 833-46  
 CODEN: LACHDL; ISSN: 0170-2041  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 OTHER SOURCE(S): CASREACT 111:154137  
 GI



AB RCH: C(CF<sub>3</sub>)<sub>2</sub> [R = CH:CCl<sub>2</sub>, CH: CMe<sub>2</sub>, CH(OEt)<sub>2</sub>], were prepared from RCHO, C12C(CF<sub>3</sub>)<sub>2</sub> and PPh<sub>3</sub> and converted into 2,2-bis(trifluoromethyl)cyclopropanecarboxylates I [R1 = OEt] by reaction with Me<sub>2</sub>S+C-HCO<sub>2</sub>Et. I [R = CHO, R1 = OEt], obtained from (EtO)<sub>2</sub>CHCH: C(CF<sub>3</sub>)<sub>2</sub> and Me<sub>2</sub>S+C-HCO<sub>2</sub>Et, is an important intermediate in the preparation of the bis(trifluoromethyl)-substituted pyrethroids I [R = CH: CBr<sub>2</sub>, CH: C(CF<sub>3</sub>)<sub>2</sub>, CH: CCl(CF<sub>3</sub>), R1 = OEt]. Hydrolysis of I (R = CH:CCl<sub>2</sub>, CHClCHMe<sub>2</sub>; R1 = OEt) gave I (R1 = OH), which were converted to pyrethroid esters I [R1 = OCH(CN)C<sub>6</sub>H<sub>4</sub>OPH-3] via I [R1 = Cl]. 4-ClC<sub>6</sub>H<sub>4</sub>CH: C(CF<sub>3</sub>)<sub>2</sub> reacts with Me<sub>2</sub>C(CN)OH to form 4-ClC<sub>6</sub>H<sub>4</sub>CH(CN)CH(CF<sub>3</sub>)<sub>2</sub>. 4-ClC<sub>6</sub>H<sub>4</sub>CH(COCl)CH(CF<sub>3</sub>)<sub>2</sub>, prepared from the nitrile via the acid, was treated with 3-PhOC<sub>6</sub>H<sub>4</sub>CH(CN)OH to give hexafluorofenvalerate, 4-ClC<sub>6</sub>H<sub>4</sub>CH(CN)CH(CF<sub>3</sub>)<sub>2</sub>CO<sub>2</sub>CH(CN)C<sub>6</sub>H<sub>4</sub>OPH-3.  
 IT 121618-14-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and cyclopropanation of, with (ethoxycarbonylmethylidene)dimethylsulfurane)  
 RN 121618-14-2 CAPLUS  
 CN 4-Hexen-3-ol, 6,6,6-trifluoro-2-methyl-5-(trifluoromethyl)-, acetate (9CI)  
 (CA INDEX NAME)

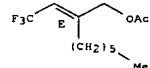
L4 ANSWER 34 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1989:212158 CAPLUS  
 DOCUMENT NUMBER: 110:212158  
 TITLE: Palladium(0)-catalyzed reactions of trifluoromethylated allylic ester derivatives: synthesis of trifluoromethylated chrysanthem acid ester  
 AUTHOR(S): Hanzawa, Yuji; Ishizawa, Seiji; Kobayashi, Yoshiro  
 CORPORATE SOURCE: Tokyo Coll. Pharm., Hachioji, 192-03, Japan  
 SOURCE: Chemical & Pharmaceutical Bulletin (1988), 36(10), 4209-12  
 CODEN: CPBTAL; ISSN: 0009-2363  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 110:212158  
 GI



AB Reactions of RCH(OAc)CR1:CR2CF<sub>3</sub> (R = PhCH<sub>2</sub>CH<sub>2</sub>, H; R1 = hexyl, H; R2 = octyl, H), PhCH<sub>2</sub>CH<sub>2</sub>CH(OAc)C(CF<sub>3</sub>)CH<sub>2</sub> and CF<sub>3</sub>CH(OAc)CH:CH:CR4R5 (R3 = Ac, CO<sub>2</sub>Et, P(O)(OEt)<sub>2</sub>, SO<sub>2</sub>C<sub>6</sub>H<sub>4</sub>Me-4; R4, R5 = H, hexyl] with NaCH(CO<sub>2</sub>Me)<sub>2</sub> in the presence of palladium catalyst, e.g., (Ph<sub>3</sub>P)<sub>4</sub>Pd, and their use in synthesizing trifluoromethylated chrysanthem acids I are described. Thus, CF<sub>3</sub>CH(OAc)CH:CH:CHMe<sub>2</sub>CO<sub>2</sub>Ac heated with NaCH(CO<sub>2</sub>Me)<sub>2</sub> in THF in the presence of (Ph<sub>3</sub>P)<sub>4</sub>Pd to give CF<sub>3</sub>CH(OAc)CH:CH:CHMe<sub>2</sub>CH(CO<sub>2</sub>Me)<sub>2</sub>, which was treated with DBU in the presence of bis(1,2-bis(diphenylphosphino)ethane)palladium to give 73% cyclopropanedicarboxylate II. Treating II with NaCH in Me<sub>2</sub>SO gave 47% I.  
 IT 120596-30-7 120596-31-8 120596-32-9  
 120596-33-0 120596-34-1 129049-09-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (substitution reaction of, with malonate in presence of palladium)  
 RN 120596-30-7 CAPLUS  
 CN 1-Octanol, 2-(2,2,2-trifluoroethylidene)-, acetate, (E)- (9CI) (CA INDEX NAME)

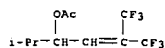
Double bond geometry as shown.



RN 120596-31-8 CAPLUS  
 CN 2-Undecen-1-ol, 3-(trifluoromethyl)-, acetate, (E)- (9CI) (CA INDEX NAME)

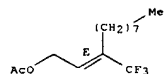
10539639a.trn

L4 ANSWER 33 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



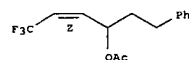
L4 ANSWER 34 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Double bond geometry as shown.



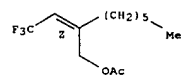
RN 120596-32-9 CAPLUS  
 CN Benzenepropanol, α-(3,3,3-trifluoro-1-propenyl)-, acetate, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



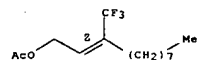
RN 120596-33-0 CAPLUS  
 CN 1-Octanol, 2-(2,2,2-trifluoroethylidene)-, acetate, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



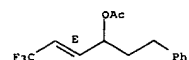
RN 120596-34-1 CAPLUS  
 CN 2-Undecen-1-ol, 3-(trifluoromethyl)-, acetate, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 129049-09-8 CAPLUS  
 CN Benzenepropanol, α-(3,3,3-trifluoro-1-propenyl)-, acetate, (E)- (9CI) (CA INDEX NAME)

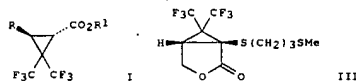
Double bond geometry as shown.



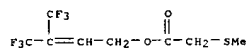
L4 ANSWER 34 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSWER 35 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1986:423961 CAPLUS  
 DOCUMENT NUMBER: 105:23961  
 TITLE: Stereoselective synthesis of gem-bistrifluoromethylcyclopropane derivatives  
 AUTHOR(S): Taguchi, Takeo; Hosoda, Akihiko; Torisawa, Yutaka; Shimazaki, Akimori; Kobayashi, Yoshiro; Tashima, Kazunori  
 CORPORATE SOURCE: Tokyo Coll. Pharm., Hachioji, 192-03, Japan  
 SOURCE: Chemical & Pharmaceutical Bulletin (1985), 33(9), 4085-7  
 CODEN: CPBTAL; ISSN: 0009-2363  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 105:23961  
 GI



AB The trans-bis(trifluoromethyl)cyclopropanecarboxylate I (R = CH2OEt, R1 = Et) (II) was prepared in 44% yield by treating (CF3)2C:CHR with Me2S-C-HCO2Et. II was further converted to I (R = CH2Cl; R1 = (NC)CHC6H4OPh-3) in 8 steps. The cis-derivative III was prepared in 43% yield by treating (CF3)2C:CHCH2O2CCH(SR2)2 [R2 = (CH2)3] with CF3SO3Me followed by KF and 18-crown-6 in CH2Cl2-DMP.  
 IT 102710-53-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation and reaction of, with benzenethiol)  
 RN 102710-53-2 CAPLUS  
 CN Acetic acid, (methylthio)-, 4,4,4-trifluoro-3-(trifluoromethyl)-2-butenyl ester (9C1) (CA INDEX NAME)



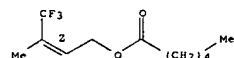
L4 ANSWER 36 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1985:57745 CAPLUS  
 DOCUMENT NUMBER: 102:57745  
 TITLE: Design of novel insect anti-juvenile hormones: allylic alcohol derivatives  
 AUTHOR(S): Quistad, Gary B.; Cerf, David C.; Kramer, Steven J.; Bergot, B. John; Schooley, David A.  
 CORPORATE SOURCE: Dep. Biochem. Insect Res., Zeecon Corp., Palo Alto, CA, 94304, USA  
 SOURCE: Journal of Agricultural and Food Chemistry (1985), 33(1), 47-50  
 CODEN: JAFCAU; ISSN: 0021-8561  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Three analogs of 3,3-dimethyl-2-propenol (dimethylallyl alc.) were synthesized and found to possess antijuvenile hormone activity when assayed on lepidopteran species (particularly the tobacco hornworm, Manduca sexta). The most active compound of those described, 3,3-dichloro-2-propenyl hexanoate [93404-30-9], caused precocious metamorphosis, inhibited juvenile hormone (JH) biosynthesis in vitro, and reduced JH titers in vivo.

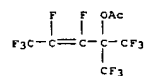
IT 93404-31-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and antijuvenile hormone activity of)  
 RN 93404-31-0 CAPLUS  
 CN Hexanoic acid, 4,4,4-trifluoro-3-methyl-2-butenyl ester, (Z)- (9C1) (CA INDEX NAME)

Double bond geometry as shown.



L4 ANSWER 37 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1971:517925 CAPLUS  
 DOCUMENT NUMBER: 75:117925  
 TITLE: Preparation and reactions of some carbinols containing the pentafluoropropenyl group  
 AUTHOR(S): Tarrant, Paul; Whitfield, Ralph W., Jr.; Summerville, Richard H.  
 CORPORATE SOURCE: Dep. Chem., Univ. Florida, Gainesville, FL, USA  
 SOURCE: Journal of Fluorine Chemistry (1971), 1(1), 31-40  
 CODEN: JFLCAR; ISSN: 0022-1139  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB 1,1,1,2,3,3-Hexafluoropropane was dehydrofluorinated to yield a 1:1 mixture of (Z)- and (E)-1H-pentafluoropropene. This mixture reacted with BuLi to give (Z)-(pentafluoropropenyl)lithium, which reacted with carbonyl compounds to give exclusively (Z)-pentafluoropropenyl carbinols. The yields were greater than 50%, indicating that the lithium reagent does not retain its stereochem. identity at low temperature, contrary to the hydrocarbon analog. Hydrolysis of CF3CF:CFLi also gave exclusively the (Z)-fluoroolefin. Treating (Z)-CF3CF:CF(CF3)2OH with SF4 gave the E isomer. Chemical properties of the carbinols are described.  
 IT 33683-43-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 33683-43-1 CAPLUS  
 CN 3-Penten-2-ol, 1,1,1,3,4,5,5-octafluoro-2-(trifluoromethyl)-, acetate (8C1) (CA INDEX NAME)





L4 ANSWER 38 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1969:58379 CAPLUS

DOCUMENT NUMBER: 70:58379

TITLE: Perfluoroalkyl and  $\alpha$ -chloroperfluoroalkyl-3-acyloxy-1,3-butadienes and polymers

INVENTOR(S): Middleton, William J.

PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co.

SOURCE: U.S., 3 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3424732	A	19690128	US 1965-509174	19651122

PRIORITY APPLN. INFO.:

US 1965-509174 A 19651122

AB (CF<sub>3</sub>)<sub>2</sub>C(OAc)CH:CH<sub>2</sub> (I) is prepared and pyrolyzed to give (CF<sub>3</sub>)<sub>2</sub>C:CHC(OAc):CH<sub>2</sub> (II) or a polymer of II. II is also polymerized with a free radical catalyst. The polymer melts at >220° and is suitable for molding into transparent film having good flexibility and excellent solvent resistance. Thus, MeC.tpbond.CH 100, CF<sub>3</sub>COCF<sub>3</sub> 100, and hydroquinone 1 g. was heated at 150° for 48 hrs. in a bomb to give 70.5 g. (CF<sub>3</sub>)<sub>2</sub>C(OH)CH:CH<sub>2</sub>, b. 105-6°, nd<sub>D</sub> 1.3477, which (20.6 g.) was added slowly to 100 ml. MeOCH<sub>2</sub>CH<sub>2</sub>OMe containing 4.5 g. 5% NaH (in mineral oil). The mixture was cooled in an ice bath, treated slowly with 7.9 g. AcCl, and poured into 200 ml. water to give 22.2 g. I, b. 135-6°, nd<sub>D</sub> 1.3668, which (14 g.) was added during 1 hr. to a silica glass tube heated at 500° and inclined at 45°. The pyrolyzate was distilled to give 8 g. II, b<sub>D</sub> 22 66-8°. II was polymerized at 60-90° in the presence of [Me<sub>2</sub>C(CN)N:]<sub>2</sub> or Bz<sub>2</sub>O<sub>2</sub>. I was also converted to the polymer of II by pyrolysis at 500° in a Pt tube followed by heating at 80-100°.

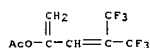
IT 20227-71-8P 28157-84-8P

RL: PREP (Preparation)

(preparation of)

RN 20227-71-8 CAPLUS

CN 1,3-Pentadien-2-ol, 5,5,5-trifluoro-4-(trifluoromethyl)-, acetate (8CI) (CA INDEX NAME)



RN 28157-84-8 CAPLUS

CN 1,3-Pentadien-2-ol, 5,5,5-trifluoro-4-(trifluoromethyl)-, acetate, polymers (8CI) (CA INDEX NAME)

CM 1

L4 ANSWER 39 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1968:86600 CAPLUS

DOCUMENT NUMBER: 68:86600

TITLE: Rearrangement of esters in the gas phase. II. Substituent effects on the rate of isomerization of allylic esters

AUTHOR(S): Lewis, Edward Sheldon; Hill, James Theo; Newman, Edward R.

CORPORATE SOURCE: Rice Univ., Houston, TX, USA

SOURCE: Journal of the American Chemical Society (1968), 90(3), 662-8

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The rearrangement of  $\alpha$ - and  $\gamma$ -trifluoromethylallyl trifluoroacetates, allyl-u-d<sub>2</sub> trifluoroacetate, allyl trifluoroacetate-18O,  $\alpha$ , $\beta$ -dimethylallyl acetate, and  $\alpha$ , $\gamma$ -dimethylallyl acetate was studied. In some cases a minor but detectable rearrangement to cis- as well as trans- $\gamma$ -substituted allyl derivs. was observed. The rate of rearrangement of allyl acetate was within exptl. error the same whether followed by D or 18O labeling. The results were consistent with a transition state with carbonium carboxylate character. 21 references.

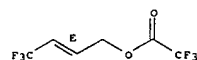
IT 19235-03-1 19235-04-2

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent) (rearrangement of, kinetics of)

RN 19235-03-1 CAPLUS

CN Acetic acid, trifluoro-, 4,4,4-trifluoro-2-butenyl ester, (E)- (8CI) (CA INDEX NAME)

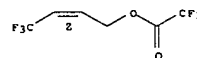
Double bond geometry as shown.



RN 19235-04-2 CAPLUS

CN Acetic acid, trifluoro-, 4,4,4-trifluoro-2-butenyl ester, (Z)- (8CI) (CA INDEX NAME)

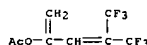
Double bond geometry as shown.



L4 ANSWER 38 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CRN 20227-71-8

CMF C8 H6 F6 O2



L4 ANSWER 40 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1966:490634 CAPLUS

DOCUMENT NUMBER: 65:90634

ORIGINAL REFERENCE NO.: 65:16962f-g

TITLE: Addition reactions of nitroso groups. Diene syntheses of nitrosobenzenes with 2-substituted 1,3-butadienes

AUTHOR(S): Kresze, G.; Korpiun, O.

CORPORATE SOURCE: Tech. Hochsch., Munich, Germany

SOURCE: Tetrahedron (1966), 22(8), 2493-504

CODEN: TETRAH; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 65:90634

G1 For diagram(s), see printed CA Issue.

AB Nitrosobenzenes add to 2-substituted butadienes to give, in most cases, 4-substituted 3,6-dihydro-1,2-oxazines (I). The structure of these adducts is proved by N.M.R. spectroscopy and chemical means. The kinetics of the Diels-Alder reaction of 2-arylbutadienes with p-chloronitrosobenzene was studied.

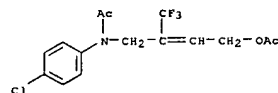
IT 7624-71-7P, Acetanilide, 4'-chloro-N-[4-hydroxy-2-(trifluoromethyl)-2-butenyl]-, acetate 7624-73-9P, Acetanilide, 4'-chloro-N-[4-hydroxy-2-(trifluoromethyl)-2-butenyl]-, trifluoroacetate

RL: PREP (Preparation)

(preparation of)

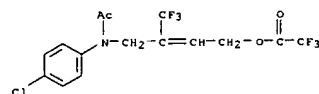
RN 7624-71-7 CAPLUS

CN Acetanilide, 4'-chloro-N-[4-hydroxy-2-(trifluoromethyl)-2-butenyl]-, acetate (7CI, 8CI) (CA INDEX NAME)

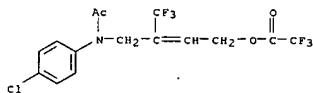


RN 7624-73-9 CAPLUS

CN Acetic acid, trifluoro-, ester with 4'-chloro-N-[4-hydroxy-2-(trifluoromethyl)-2-butenyl]acetanilide (7CI, 8CI) (CA INDEX NAME)



L4 ANSWER 41 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1966:490633 CAPLUS  
 DOCUMENT NUMBER: 65:90633  
 ORIGINAL REFERENCE NO.: 65:16962d-f  
 TITLE: Amino alcohols. XXIV. 4-Methyl- and 4-cyclohexylmorpholine-2,4-dione  
 Drefahl, Guenther; Hartmann, Mntred; Skurk, Axel  
 AUTHOR(S): Univ. Jena, Germany  
 CORPORATE SOURCE: Chemische Berichte (1966), 99(8), 2716-17  
 SOURCE: CODEN: CHBEAM; ISSN: 0009-2940  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 OTHER SOURCE(S): CASREACT 65:90633  
 AB cf. CA 64, 19600c; 65, 10472e. H<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>OH (30.5 g.) added dropwise at 0° with stirring to 270 cc. (CO<sub>2</sub>Et)<sub>2</sub> in 50 cc. EtOH yielded 42% HOCH<sub>2</sub>CH<sub>2</sub>NHCOCOC<sub>2</sub>Et, b<sub>0.001</sub> 155-60°, n<sub>D</sub>20 1.4724. The distillation residue recrystd. from EtOH gave an amorphous, polymeric oxamidic acid ester, m. 155-60°. BrCH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub>·HBr (41 g.) in 100 cc. absolute EtOH was treated at 0° with 50 cc. 4N alic. KOH, filtered, and added dropwise to 135 cc. (CO<sub>2</sub>Et)<sub>2</sub> in 50 cc. EtOH to give 44% BrCH<sub>2</sub>CH<sub>2</sub>NHCOCOC<sub>2</sub>Et, m. 56° (C<sub>6</sub>H<sub>6</sub>). MeNHCH<sub>2</sub>CH<sub>2</sub>OH (40 g.) in 100 cc. EtOH added dropwise at 0-5° to 100 cc. (CO<sub>2</sub>Et)<sub>2</sub> in 20 cc. EtOH and refluxed 10 min. yielded 37% 4-methylmorpholine-2,3-dione (II), m. 98-9° (C<sub>6</sub>H<sub>6</sub>). The filtrate gave 30% HOCH<sub>2</sub>CH<sub>2</sub>NHCOCOC<sub>2</sub>Et, b<sub>0.18</sub> 102-6°, n<sub>D</sub>20 1.7458. A mixture of 3.6 g. 2-cyclohexylaminoethanol in 10 cc. EtOH and 5 cc. (CO<sub>2</sub>Et)<sub>2</sub> was refluxed 0.5 hr. to yield 84% 4-cyclohexyl analog of I, m. 123-3.5° (MePh).  
 IT 7624-73-9P, Acetic acid, trifluoro-, ester with 4'-chloro-N-[4-hydroxy-2-(trifluoromethyl)-2-butenyl]acetanilide  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 7624-73-9 CAPLUS  
 CN Acetic acid, trifluoro-, ester with 4'-chloro-N-[4-hydroxy-2-(trifluoromethyl)-2-butenyl]acetanilide (7CI, 8CI) (CA INDEX NAME)

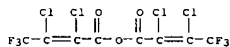


L4 ANSWER 42 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1959:56049 CAPLUS  
 DOCUMENT NUMBER: 53:56049  
 ORIGINAL REFERENCE NO.: 53:10039f-i, 10040a  
 TITLE: Dichlorotrifluorocrotonic acid  
 INVENTOR(S): Baranaukas, Charles F.; Ashton, Wm. E.  
 PATENT ASSIGNEE(S): Hooker Chemical Corp.  
 DOCUMENT TYPE: Patent  
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US 2863906		19581209	US 1955-516304	19550617

AB CF3CCl:CClCCl3 (1412 g.) (C.A. 52, 14649a) and 1567 g. H<sub>2</sub>SO<sub>4</sub> was heated at 130° 10 hrs., cooled and 500 ml. H<sub>2</sub>O added. The lower layer was extracted with 10% NaOH solution. Addition of excess HCl, extraction with Et<sub>2</sub>O, and distillation gave 780 g. CF<sub>3</sub>CCl:CClCO<sub>2</sub>H (II), b<sub>11</sub> 83-5°; 81 g. I was obtained from the H<sub>2</sub>SO<sub>4</sub> layer. Addition of 391 g. PhCCl<sub>3</sub> to 313.5 g. I at 135° followed by 0.5 hr. at 170° gave 281 g. CF<sub>3</sub>CCl:CClCOC<sub>2</sub> (III), b. 113-15°. Distillation of 104.5 g. I from 71 g. P<sub>2</sub>O<sub>5</sub> and redistn. from 15 g. P<sub>2</sub>O<sub>5</sub> gave 55 g. (CF<sub>3</sub>CCl:CClCO)<sub>2</sub>, b<sub>11</sub> 103-4°. II and ROH gave the following esters (R, b.p./mm., n<sub>D</sub>20, and % yield given): Me, 141-3°/743, 1.4103, 71; Et, 155-6°/742, 1.4108, 76; Bu, 193°/746, 1.4188, 60; Am, 207-10°/746, 1.4221, 89; n-C<sub>8</sub>H<sub>17</sub>, 134°/13, 1.4310, 50; iso-Pr, 165°/760, 1.4097, 82; CF<sub>3</sub>CH<sub>2</sub>, 145-6°/735, 1.3780, 82; tert-Bu, 65-6°/12, 1.4122, 30; CH<sub>2</sub>:CHCH<sub>2</sub>, 170-2°/760, 1.4264, 43; tetrahydrofuryl, 143-5°/30, 1.4457, 55; Ph, 113-15°/13, 1.4832, 49; cyclohexyl, 75-7°/2.5, 1.4468, 68; methylcyclohexyl, 79-81°/2.2, 1.4460, 46; -CH<sub>2</sub>CH<sub>2</sub>-, 163-4°/22, 1.4410, 81; -CH<sub>2</sub>CHMe-, 159°/13, 1.4396, 56; -(CH<sub>2</sub>)<sub>4</sub>-, 148-56°/3, 1.4439, 42; -CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>-, 189-90°/13, 1.4446, 43. Amines and II gave amides (amine, b.p./mm., and n<sub>D</sub>20 of amide given): NH<sub>3</sub> (III), -, - (m. 123-5°); BuNH<sub>2</sub>, 167-8°/30, 1.4465; PhCH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub>, -, - (m. 97-8°); (Me<sub>2</sub>CH)<sub>2</sub>NH, 134-6°/26, 1.4462; Bu<sub>2</sub>NH, -, -, 1.4510; PhNH<sub>2</sub>, -, - (m. 102-8°); H<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub>, -, - (m. 241-2°). Distillation of 31.2 g. III from 42.6 g. P<sub>2</sub>O<sub>5</sub> at mild vacuum gave 11.5 g. CF<sub>3</sub>CCl:CClCN, b. 107-8°. I and esters are useful as anthelmintic agents. Salts prepared by evaporation of solns. of I and metal carbonates are useful as grease thickeners. Amides are insect repellents.  
 IT 654-24-0, Crotonic acid, 2,3-dichloro-4,4,4-trifluoro-, anhydride (and esters)  
 RN 654-24-0 CAPLUS  
 CN 2-Butenoic acid, 2,3-dichloro-4,4,4-trifluoro-, anhydride (9CI) (CA INDEX NAME)

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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

222.28

395.51

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-32.76

-32.76

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